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University of Alberta

A Heisenberg Approach to the Quantum Fermi–Ulam Accelerator

By

William A. Atkinson

A dissertation

presented to the Faculty of Graduate Studies and Research

in partial fulfilment of the requirements for the degree

of

Masters of Science

in

Theoretical Physics

Department of Physics

Edmonton, Alberta

Spring 1992

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UNIVERSITY OF ALBERTA

FACULTY OF GRADUATE STUDIES AND RESEARCH

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance, a thesis entitled "A Heisenberg Approach to the Quantum Fermi–Ulam Accelerator" submitted by William A. Atkinson in partial fulfilment of the requirements for the degree of Masters of Science in Theoretical Physics

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Abstract

The classical Fermi–Ulam Accelerator was originally introduced as a simple time dependent system for studying the transition from classical to statistical mechanics. It consists of a particle trapped between two rigid walls, one of which moves in some prescribed manner. The particle bounces elastically from the walls and will gain or lose energy with each collision with the moving wall. Recently, a quantum version of the system has been introduced. The main object of studies involving the quantum Accelerator has been to examine the transition from quantum to classical mechanics in a simple time dependent system. This thesis looks at a formulation of the quantum Accelerator from within the framework of the Heisenberg picture. Along the way to formulating the problem, a detailed examination of the quantum particle-in-a-box problem is made.

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Chapter 1

Introduction

In 1949, Fermi [1], proposed a model for a cosmic radiation source. At that time, there were several unanswered questions concerning cosmic rays; it was not understood how any known source could produce particles of such high energy with such great intensity. Fermi proposed the following: giant molecular clouds, ionized sufficiently for a magnetic field to be trapped in the cloud, could transfer tremendous amounts of energy to charged particles interacting with the magnetic field. The process consisted of a series of collisions between the particles and the randomly moving clouds. Fermi felt that, overall, there would be a net transfer of momentum to the particles and that, given enough time, the particles would attain very high energies. The sheer size of the clouds would account for the intensity of observed radiation.

Similar models were studied by Ulam [2]. He examined several systems—such as gravitational 3–body systems and n–particle systems with elastic collisions—with the intention of understanding the transition from classical to statistical mechanics. The most well known system which he examined is now called the Fermi–Ulam Accelerator. It consists of two walls (usually infinitely massive) which move with respect to one another, and a particle trapped between them. The particle collides (usually elastically) with the walls and will either gain or lose energy during the collision depending on whether the wall and particle are moving towards or away from one another at the time of collision. Ulam performed numerical simulations of this system and was surprised not to find the kind of energy growth predicted by statistical arguments.

The contradiction between the theoretical work of Fermi and Ulam and the numerical work of Ulam provoked many detailed studies of the phase space over the next decade. Numerical and theoretical work by Zaslavskiĭ and Chirikov [3, 4], Brahic [5] and Lichtenberg and Lieberman [6], revealed that the Fermi–Ulam Accelerator only follows statistical laws in some regions of phase space, and that the energy growth proposed by Ulam and Fermi is limited by the size of the stochastic regions.

The complicated nature of the phase space of the Fermi–Ulam Accelerator has made it a useful model for demonstrating many aspects of classical behaviour for more than thirty years. Oddly, though, the natural transition to the quantum Fermi–Ulam Accelerator has only been made recently. Its study has been prompted, to a large extent, by interest in quantum chaology—the study of quantum systems whose classical counterparts exhibit stochastic behaviour. The bulk of the work in this field has been with time independent systems. The first of the time dependent systems to be seriously studied was the kicked quantum rotor (consisting of a periodically forced rotating system for which the forcing function is composed of a series of delta–function kicks)[7]. The quantum Fermi–Ulam Accelerator, introduced in 1986 by José and Cordery [8], is the second time dependent system to receive widespread study.

Time dependent quantum systems have a number of experimental applications as well as the purely theoretical ones described above. One of the most interesting applications is to electromagnetic traps, which are mathematically similar to the quantum Fermi–Ulam Accelerator. Two thirds of the 1989 Nobel Prize in Physics was awarded to Dehmelt and Paul [9, 10] for their contribution to the physics of single particle systems. In one experiment, Dehmelt was able to store a single electron in a trap for ten months in order to study its structure. One of the most fascinating aspects of this work is that it allows direct observations of the single particle quantum wavefunction; virtually all other experiments can only provide statistical results from a very large number of quantum particles. These kinds of experimentally realised

single particle quantum systems have made theoretical studies of similar systems (such as the quantum Fermi–Ulam Accelerator) extremely interesting; they provide a motivation for studying different time dependent models and an opportunity to confirm the results.

Obtaining a description of the quantum behaviour of any system is the first goal of most studies of time dependent systems. The second goal is usually to understand the correlation between the quantum and classical behaviour. The second goal forms the basis of quantum chaology [7]. The aim of this thesis was originally to address these two problems. However, as work progressed it became apparent that a thorough understanding of the formulation of the problem is crucial, and a large portion of the thesis is dedicated to this topic. The thesis is ordered as follows: Chapter 2 of the thesis is a short description of the classical problem. Chapter 3 contains a description of several approaches to the quantum Fermi–Ulam Accelerator, followed by a discussion of the discrepancies which occur between two of the approaches. Chapter 4 consists of a very careful treatment of the operators needed to describe the quantum problem, with the aim of resolving the discrepancies mentioned in chapter 3. Chapter 5 is a brief discussion the the semiclassical limit. Chapter 6 contains both a solution to the Heisenberg equations for a special case of the Fermi–Ulam Accelerator in which the wall motion is linear and a discussion of an alternative formulation of the problem. Chapter 7, the conclusion, contains a summary of the results of the thesis as well as a discussion of the work which next needs to be done.

Chapter 2

Classical Theory

A Fermi–Ulam Accelerator is usually constructed as follows[2]: Fixed rigid walls are placed at $x = 0$ and at $x = L(t)$, t being time. A ball bounces elastically between the walls. The position of the ball is denoted by $x(t)$. The ball moves freely between the walls and the bounces are given by the following boundary conditions: when $x = 0$ then $p \rightarrow -p$ and when $x = L(t)$ then $p \rightarrow -p + 2m\dot{L}$ (m is the mass of the particle, p is the momentum and the overdot denotes differentiation with respect to time). The behaviour of the system is usually discussed in terms of the values of p, x and t at the n^{th} bounce from the moving wall.

The time between two successive bounces from the moving wall is

$$t_{n+1} - t_n = \frac{m}{\mid p_n \mid}[L(t_n) + L(t_{n+1})]. \tag{2.1}$$

Here p_n is the momentum of the ball *after* the n^{th} bounce from the moving wall and it is always negative:

$$p_n = p_{n-1} + 2m\dot{L}(t_n). \tag{2.2}$$

The position at the n^{th} bounce is simply:

$$x_n = L(t_n). \tag{2.3}$$

Equations 2.1 and 2.2 form a set of difference equations which (except for a few simple cases) cannot be explicitly solved. Equation 2.3 follows trivially.

A wall motion for which the transcendental nature of 2.1 is removed is formed

from a piecewise connection of wall motions of the form

$$L(t) = \sqrt{At^2 + Bt + C}, \tag{2.4}$$

for which 2.1 and 2.2 become

$$t_{n+1} = \frac{B + [A + (p_n/m)^2]t_n + 2(\mid p_n \mid /m)\sqrt{At_n^2 + Bt_n + C}}{(p_n/m)^2 - A} \tag{2.5}$$

and

$$p_n = p_{n-1} + 2m\frac{At_n + B/2}{\sqrt{At_n^2 + Bt_n + C}} \tag{2.6}$$

The interesting feature of this case is that it is the most general type of wall motion for which the quantum version of the problem has been solved.

The kinds of wall motions used by other authors include special cases of 2.4, such as connected segments of linear wall motion [11, 12] and connected segments with $A = 0$ [13], as well as more general motions such as connected segments with linearly changing wall velocity ($L(t) = At^2 + Bt + C$) [3, 4] and even sinusoidal variations [14]. In general, the simpler forms of wall motion allow a more accurate treatment of the behaviour and the more complicated (eg. sinusoidal) motions require approximations which necessarily limit the scope of the work.

The classical system has proven interesting for two reasons. The first reason is that it is an excellent model of a time dependent system that exhibits stochastic and regular behaviour. The original proposal, by Fermi [1], of the possibility of unbounded energy growth led to more detailed explorations of the phase space [2, 3, 4, 13, 6]. The problem is well studied and the conclusions can be summarised: There is a finite upper bound to the energy which any particle can gain in a periodic Fermi–Ulam Accelerator [15]. Furthermore, for particles with high enough initial energies, there are also bounds on the amount of energy which can be lost. In general there are three regions of phase space:

1. Low particle velocities for which the motion is stochastic.

2. Intermediate particle velocities for which islands of stability are contained in an otherwise stochastic phase space.

3. High particle velocities for which the motion is regular and the energy oscillates about a mean value with the period of the walls. In this limit the wall motion is adiabatic relative to the particle motion.

A second reason for studying the classical system is to understand the transition from quantum to classical systems [11, 16, 7]. This is a poorly developed area of theory which will be discussed in detail in a later chapter.

Chapter 3

Quantum Theory

The classical system is usually quantised [13, 11, 12, 8, 17, 18] in the following manner: the Hamiltonian which generates free particle behaviour is

$$\hat{H} = \hat{p}^2/(2m), \tag{3.1}$$

where the $\hat{}$ is used to denote operators. It is usually assumed that the classical 'bounce' boundary conditions correspond to Dirichlet boundary conditions on the quantum wavefunction:

$$\Psi(x = 0, t) = \Psi(x = L(t), t) = 0. \tag{3.2}$$

The Schrödinger equation becomes

$$-(\hbar^2/2m)\partial_x^2\Psi = i\hbar\partial_t\Psi \tag{3.3}$$

where ∂_x denotes the partial derivative with respect to x. This is nonseparable because of the boundary conditions. For numerical studies [13, 8] the wavefunction is traditionally expanded in terms of instantaneous eigenstates, $\phi_n(x, t)$, of the Hamiltonian:

$$\phi_n = (-1)^n[2/L(t)]^{1/2}\sin[n\pi x/L(t)], \tag{3.4}$$

and the time evolution of the expansion coefficients is calculated.

This is not a useful approach for analytical studies, however, and a more recently developed approach is becoming standard [11, 12, 16, 19, 17, 18]. The nonseparability of the boundary conditions can be removed by the sequence of unitary

transformations given by

$$\hat{U}_1 \equiv exp[-\frac{i}{2\hbar}(\hat{x}\hat{p}+\hat{p}\hat{x})\log(L(t))] \tag{3.5}$$

and

$$\hat{U}_2 \equiv exp[\frac{i}{2\hbar}mL\dot{L}\hat{x}^2]. \tag{3.6}$$

Along with the commutation rule

$$[\hat{x},\hat{p}] = i\hbar, \tag{3.7}$$

$\hat{U}_1$ has the following effect:

$$\begin{aligned} \hat{U}_1^{-1}\hat{p}\hat{U}_1 &= \hat{p}/L(t) \\ \hat{U}_1^{-1}\hat{x}\hat{U}_1 &= \hat{x}L(t) \end{aligned} \tag{3.8}$$

and 3.3 transforms into

$$-\frac{\hbar^2}{2mL^2}\partial_x^2\Psi = i\hbar\partial_t\Psi + \frac{\dot{L}}{2L}(\hat{x}\hat{p}+\hat{p}\hat{x})\Psi. \tag{3.9}$$

Because the same notation is being used for the operators before and after the transformation, it is important to understand the meaning of 3.8. The effect of $\hat{U}_1^{-1}$ on a function is

$$\hat{U}_1^{-1}f(x) = \sqrt{L(t)}\, f(xL(t)) \tag{3.10}$$

so that the boundary conditions now become

$$\hat{U}_1^{-1}\Psi(x=0) = \Psi(xL(t)=0) = \Psi(x=0) = 0 \tag{3.11}$$

$$\hat{U}_1^{-1}\Psi(x=L(t)) = \Psi(xL(t)=L(t)) = \Psi(x=1) = 0. \tag{3.12}$$

$\hat{U}_1$ scales the interval $[0, L(t)]$ into the interval $[0, 1]$. $\hat{U}_2$ is introduced to eliminate the crossterms in 3.9:

$$\hat{U}_2^{-1}\hat{U}_1^{-1}\hat{p}\hat{U}_1\hat{U}_2 = \hat{p}/L(t) + \hat{x}m\dot{L}(t) \tag{3.13}$$

$$\hat{U}_2^{-1}\hat{U}_1^{-1}\hat{x}\hat{U}_1\hat{U}_2 = \hat{x}L(t) \tag{3.14}$$

and 3.9 becomes

$$-\frac{\hbar^2}{2mL^2}\partial_x^2\Psi + \frac{m}{2}L\ddot{L}x^2\Psi = i\hbar\partial_t\Psi \tag{3.15}$$

It is often convenient to rescale the time in 3.15 so that

$$\tau \equiv \int^t \frac{ds}{L^2(s)} \tag{3.16}$$

and 3.15 becomes

$$-\frac{\hbar^2}{2m}\partial_x^2\Psi + \frac{m}{2}g(\tau)x^2\Psi = i\hbar\partial_t\Psi \tag{3.17}$$

with

$$g(\tau) = [(1/L)d_\tau^2 L - (2/L^2)(d_\tau L)^2]. \tag{3.18}$$

The boundary conditions are not affected by $\hat{U}_2$ and are still given by 3.11 and 3.12.

It is easily shown that if $L(t)$ is periodic, with period T, then $g(\tau)$ is also periodic with period $\tilde{T} = \tau(T)$. Under such circumstances, 3.17 is known to have solutions of Floquet type [20]: $\Psi(\tau) = \hat{U}(\tau)\Psi(0)$, where $\hat{U}(\tau)$ is a time evolution operator with the form

$$\hat{U}(\tau) = \hat{P}(\tau)e^{-\frac{i}{\hbar}\hat{M}\tau} \tag{3.19}$$

and $\hat{P}(\tau)$ is periodic with period $\tilde{T}$. Further, $\hat{P}(\tau = 0) = \hat{I}$, the identity operator. $\hat{M}$ is a time independent, self adjoint operator. The one cycle evolution operator is defined as

$$\hat{U} \equiv \hat{U}(\tilde{T}) = e^{-\frac{i}{\hbar}\hat{M}\tilde{T}}. \tag{3.20}$$

After n cycles of wall motion the time evolution operator is just

$$\hat{U} \equiv \hat{U}(n\tilde{T}) = \hat{U}^n \tag{3.21}$$

so that the time evolution of a system may be discussed in terms of the relatively simple operator, $\hat{U}$. It is this approach that Seba [12] takes when he discusses the boundedness of the quasienergy of a quantum particle. The technique he uses is quite general and follows the work of [21].

The argument depends on the self adjointness of $\hat{M}$, which guarantees the existence of a complete set of orthogonal eigenfunctions spanning the Hilbert space, provided the eigenvalues are discrete [20]. Denoting the eigenfunctions by ψ_n and the eigenvalues by λ_n, an arbitrary wavefunction may be expanded in terms of these states [21]:

$$\begin{aligned} \Psi(\tau) &= \sum_n a_n \hat{P}(\tau) e^{-\frac{i}{\hbar}\hat{M}\tau}\psi_n \\ &= \sum_n a_n e^{-\frac{i}{\hbar}\lambda_n \tau}\hat{P}(\tau)\psi_n \end{aligned} \tag{3.22}$$

so that the quasi-energy expectation value is

$$\langle\Psi(\tau)|i\hbar\partial_\tau|\Psi(\tau)\rangle = \sum_{m,n} a_n^* a_m e^{-\frac{i}{\hbar}(\lambda_m-\lambda_n)\tau}[\lambda_m\delta_{m,n} + \langle\psi_n|\hat{P}^\dagger(\tau)i\hbar\partial_\tau\hat{P}(\tau)|\psi_m\rangle], \tag{3.23}$$

where † denotes Hermitian conjugate. The infinite sum in 3.23 can be broken into a finite sum

$$\sum_{m,n=1}^{N} a_n^* a_m e^{-\frac{i}{\hbar}(\lambda_m-\lambda_n)\tau}[\lambda_m\delta_{m,n} + \langle\psi_n|\hat{P}^\dagger(\tau)i\hbar\partial_\tau\hat{P}(\tau)|\psi_m\rangle]$$

and an infinite sum,

$$\sum_{m,n=N+1}^{\infty} a_n^* a_m e^{-\frac{i}{\hbar}(\lambda_m-\lambda_n)\tau}[\lambda_m\delta_{m,n} + \langle\psi_n|\hat{P}^\dagger(\tau)i\hbar\partial_\tau\hat{P}(\tau)|\psi_m\rangle].$$

The infinite sum can be made arbitrarily small by choosing N large enough, since $a_n \to 0$ in the large-n limit (this is necessary for 3.22 to be normalised). The approximation made to 3.22 by the finite sum will be recurrent in the sense that it will come arbitrarily close to its initial value infinitely many times over the course of its evolution. The remaining infinite sum will not change this, because of its arbitrarily small nature. Unbounded energy growth is not possible in recurrent systems. Of course, this will break down if the spectrum, λ_n, contains a continuous component—in which case the time between recurrences becomes infinite. In such a case, unbounded energy growth may occur.

Seba's paper is, therefore, devoted to demonstrating the discrete nature of the quasienergy spectrum. His condition for boundedness is that $L(t)$ be five times differentiable, though failure to meet this requirement does not necessarily imply unbounded behaviour.

Seba also gives an example of, and a criterion for, unbounded energy growth through a quantum resonance. Periodic wall motion which is continuous in time but which has occasional discontinuities in its derivative will provide a series of delta-function kicks to the system; $g(\tau)$ will have the form

$$\begin{aligned} g(\tau) &= g_0(\tau) + \alpha_0 \sum_n \delta(\tau - \tau_0 - n\tilde{T}) + \alpha_1 \sum_n \delta(\tau - \tau_1 - n\tilde{T}) \\ &\quad + \ldots + \alpha_j \sum_n \delta(\tau - \tau_j - n\tilde{T}) \end{aligned} \tag{3.24}$$

$$\tag{3.25}$$

where g_0 is a piecewise continuous, periodic function, and there are j discontinuities over the course of one period of wall motion. The strengths of the discontinuities are α_i. Seba's condition for resonant growth due to the δ–kicks is that

$$\int_0^T \frac{dt}{[L(t)]^2} = p/q\pi, \ p, q \text{ are integer.} \tag{3.26}$$

This kind of resonance is a purely quantum effect that has no classical counterpart. It is one of the most dramatic consequences of the differences between quantum and classical mechanics because it survives into the realm of the large energy limit, which is often taken to be a classical limit.

There are not many exact solutions for the quantum Fermi–Ulam Accelerator. The most general exact solution is given by the case that g_0 is piecewise constant in 3.24. Solutions to 3.17 are separable and can be joined across the discontinuities. As was mentioned before, this case is given by piecewise connections of

$$L(t) = \sqrt{At^2 + Bt + C}. \tag{3.27}$$

This solution, though limited, is interesting because it is an exact solution for which the corresponding classical system exhibits both regular and stochastic behaviour. The connection between the quantum and classical solutions for this special case are discussed in detail in chapter 5.

Two unsatisfactory aspects of the work which has been described are the dependence of the results on the periodicity of the wall motion and an inability to discuss the behaviour of the solution as a continuous function of time. The second of these is particularly a problem for discussions of semiclassical physics where it is necessary to reconcile a discrete mapping over one period of wall motion (quantum picture) with a discrete mapping between consecutive bounces from the moving wall (classical picture). This is discussed in [11], and will be examined in more detail in chapter 5. An attempt at overcoming these difficulties is made by Razavy [17].

Razavy's approach is to solve the operator equations of motion generated in the Heisenberg picture by the Hamiltonian, 3.1. The Heisenberg equations of motion for an operator $\hat{A}$ are

$$i\hbar\dot{\hat{A}} = [\hat{A}, \hat{H}]. \tag{3.28}$$

With the transformations, given by $\hat{U}_1$ and $\hat{U}_2$, and the rescaling of time, given by 3.16, the equations of motion become,

$$\begin{aligned} i\hbar\, d_\tau \hat{x} &= [\hat{x}, \hat{H}] && (3.29)\\ i\hbar\, d_\tau \hat{p} &= [\hat{p}, \hat{H}] && (3.30)\\ \hat{H} &= \hat{p}^2/2m + (m/2)g(\tau)\hat{x}^2, && (3.31) \end{aligned}$$

with $g(\tau)$ given by 3.18. Along with 3.7, this becomes

$$\begin{aligned} d_\tau^2 \hat{x} + g(\tau)\hat{x} &= 0 && (3.32)\\ \hat{p} &= m\, d_\tau \hat{x}. && (3.33) \end{aligned}$$

Equations 3.32 and 3.33 are just the harmonic oscillator equations of motion with a time varying oscillator strength. The classical equations corresponding to these have been well studied and it is easily shown that the operator solutions can be written

$$\begin{aligned} \hat{x} &= \hat{x}_0 F(\tau) + \hat{p}_0 G(\tau)/m \\ \hat{p} &= \hat{x}_0 m\, d_\tau F(\tau) + \hat{p}_0 d_\tau G(\tau) \end{aligned} \tag{3.34}$$

where $F(\tau)$ and $G(\tau)$ are linearly independent solutions of the classical problem satisfying

$$\begin{aligned} F(0) &= d_\tau G(0) \\ &= 1 \end{aligned} \tag{3.35}$$

$$\begin{aligned} G(0) &= d_\tau F(0) \\ &= 0 \end{aligned} \tag{3.36}$$

Here $\hat{x}_0$ and $\hat{p}_0$ are the Heisenberg operators at $\tau = 0$ and they coincide with the Schrödinger operators so that

$$\hat{x}_0 f(x) = x f(x) \tag{3.37}$$

$$\hat{p}_0 f(x) = -i\hbar \partial_x f(x). \tag{3.38}$$

At this point it is important to realise that 3.18 can be rewritten

$$d_\tau^2 (1/L) + g(\tau)(1/L) = 0 \tag{3.39}$$

which has the same form 3.32, so that solutions of F and G are related to $(1/L)$. A second solution to 3.39 is easily shown to be

$$\Lambda(\tau) = (1/L) \int_0^\tau L^2(\tau') d\tau' \tag{3.40}$$

and F and G may be written in terms of L and Λ.

$$\begin{aligned} F(\tau) &= 1/L(\tau) - [d_\tau(1/L(\tau))]_{\tau=0}\Lambda(\tau) \\ G(\tau) &= \Lambda(\tau). \end{aligned} \tag{3.41}$$

For a physically meaningful system, $L(\tau)$ is never zero or infinite, so that Λ is an increasing function of τ.

Rewriting the Hamiltonian, 3.31, in terms of the solution, 3.34, gives:

$$\begin{aligned} \hat{H} &= (m/2)[(d_\tau F)^2 + g(\tau)F^2]\hat{x}_0^2 + (1/2m)[(d_\tau G)^2 + g(\tau)G^2]\hat{p}_0^2 \\ &\quad +(1/2)[d_\tau F d_\tau G + g(\tau)FG](\hat{x}_0\hat{p}_0 + \hat{p}_0\hat{x}_0). \end{aligned} \tag{3.42}$$

From this it is obvious that unbounded quasi–energy growth will generally occur provided that $g(\tau)$ does not asymptotically vanish. This contradicts the result of Seba but is not necessarily unphysical because $g(\tau) \to 0$ corresponds to $L(t) \to$ constant, which is certainly more physically reasonable than having periodic oscillations for all time.

What is unphysical, however, is the behaviour of $\hat{x}(\tau)$. A simple example shows that something is not correct with the solution, 3.34: A Heisenberg wavefunction chosen such that $\langle \Psi_H | \hat{p}_0 | \Psi_H \rangle = 0$ will have a position expectation value

$$\langle \hat{x} \rangle = \langle \hat{x}_0 \rangle F(\tau).$$

However, there are many $L(t)$ for which $F(\tau)$ will grow without bound, so that $\langle \hat{x} \rangle$ will leave the interval $[0, 1]$, and therefore be outside the walls of the box.

It is not obvious where the Heisenberg approach has gone wrong. The Heisenberg approach is known to be fully equivalent [22] to the Schrödinger approach. A first guess might be that the choice of Hamiltonian is wrong, but this would not explain why the *same* wrong result is not given by both approaches. The problem,

it turns out, is in working on the finite interval $[0, 1]$, and the difficulties that this introduces are discussed in the next section.

Chapter 4

The Interval $[0, 1]$

This section is a review of some of the mathematical concepts required for working on the interval $[0, 1]$, with applications to the Fermi–Ulam Accelerator [23, 24]. The aim of this chapter is to find the source of the inconsistency between the Schrödinger and Heisenberg approaches used in the last chapter. The discussion is started with a definition of the space in which the system is described. Unless otherwise stated, natural units ($\hbar = m = 1$) will be used in this chapter.

The Hilbert space, $\mathbf{H}$, used to discuss quantum mechanics on the interval $x \in [0, 1]$ is,

$$\mathbf{H} = \mathbf{L^2}[0, 1], \tag{4.1}$$

the set of square integrable functions over the interval $[0, 1]$. An inner product of two functions is defined by

$$\langle f|g\rangle = \int_0^1 dx\, f^* g \tag{4.2}$$

so that square integrability implies $\langle f|f\rangle < \infty$. The norm of a function is defined by

$$\|f\|^2 = \langle f|f\rangle. \tag{4.3}$$

A function, f, is in the domain of an operator, $\hat{A}$, if $\hat{A}f$ is defined; this is denoted $f \in \mathbf{D}(\hat{A})$.

For an operator to represent a physical quantity, it must satisfy certain requirements:

1. An operator must be Hermitian. An operator, $\hat{A}$, is Hermitian if, $\forall f, g \in \mathbf{D}(\hat{A})$,

$$\langle \hat{A} f | g \rangle = \langle f | \hat{A} g \rangle. \tag{4.4}$$

The momentum operator, $\hat{p} = -i\partial_x$ for example, will only be Hermitian if

$$f^* g|_0^1 = 0 \text{ for all } f, g \in \mathbf{D}(\hat{p}) \tag{4.5}$$

since

$$\begin{aligned} \int_0^1 f^* \hat{p} g \, dx &= -i \int_0^1 f^* \partial_x g \, dx \\ &= i \int_0^1 g \partial_x f^* \, dx - i \, f^* g|_0^1 \\ &= \int_0^1 (\hat{p} f)^* g \, dx - i \, f^* g|_0^1 . \end{aligned} \tag{4.6}$$

Hermiticity of an operator guarantees that expectation values are real.

2. A stronger condition is that an operator must be self adjoint. A Hermitian operator, $\hat{A}$, will also be self adjoint if

$$\begin{aligned} \langle f | \hat{A} g \rangle &= \langle \phi | g \rangle \Rightarrow f \in \mathbf{D}(\hat{A}) \text{ and } \hat{A} f = \phi, \\ &\forall g \in \mathbf{D}(\hat{A}); \; \phi, f \in \mathbf{H}. \end{aligned} \tag{4.7}$$

An example of a Hermitian operator which is not self adjoint is the momentum operator defined as

$$\begin{aligned} \hat{\mathcal{P}} g(x) &= -i \partial_x g(x) \\ \forall g(x) \ni g(0) &= g(1) = 0. \end{aligned} \tag{4.8}$$

This operator is obviously Hermitian, since 4.5 is true. However, it will also be true that, given $g \in \mathbf{D}(\hat{\mathcal{P}})$, $f^* g|_0^1$ will always vanish whether f is also in $\mathbf{D}(\hat{\mathcal{P}})$ or not. From this it follows directly that 4.7 is not true, and $\hat{\mathcal{P}}$ is not self adjoint. Self adjointness of operators implies the completeness of their eigenstates provided, as has been already mentioned, the eigenvalues are discrete.

The definition, 4.7, can be shown to be equivalent to the statements

$$\hat{A} \text{ is Hermitian,}$$
$$\forall f \in \mathbf{H} \exists g_{\pm} \in \mathbf{D}(\hat{A}) \ni (\hat{A} \pm i)g_{\pm} = f. \tag{4.9}$$

In other words, self adjointness means that the domain of an operator, $\hat{A}$, is large enough that $\hat{A} \pm i$ maps into the entire Hilbert space. For practical purposes, 4.9 is easier to work with than 4.7. A simple proof of 4.9 can be found in Schechter [23, Corollary 1.8.1].

3. A third condition on physically meaningful operators is that they be defined. This is not a trivial statement. A function, f, may be in $\mathbf{D}(\hat{p})$, the domain of the momentum operator, and yet $\hat{x}f$ may not be in $\mathbf{D}(\hat{p})$, so that $\hat{p}\hat{x}f$ would not be defined. The problem of defining operators is critical when combinations of operators are considered. The domain of a combination of operators can always be found by insisting that each operator map into the domain of the subsequent operator. However it is often possible to extend the domain of the resultant operator by operating on Cauchy sequences for which each of the elements is in the domain of the operator, but the limit points are outside of the domain of the operator. What is meant by this will become more obvious when some practical calculations are done.

The operators used in solving the particle–in–a–box problem can now be defined. The position operator is defined as

$$\hat{x}g = xg, \; g \in \mathbf{H} \tag{4.10}$$

This is obviously Hermitian. Further, given any function, $f \in \mathbf{H}$,

$$\begin{aligned} (\hat{x} \pm i)g_{\pm} &= f \\ \Rightarrow g_{\pm} &= f/(x \pm i) \end{aligned} \tag{4.11}$$

and $g_\pm \in \mathbf{D}(\hat{x})$. From 4.9 it follows that $\hat{x}$ is self adjoint.

The momentum operator is defined as

$$\begin{aligned} \hat{p}f(x) &= -i\partial_x f(x) \\ \text{where } f(0) &= e^{i\theta} f(1). \end{aligned} \tag{4.12}$$

Here, θ is a fixed constant and there are an infinite number of definitions of $\hat{p}$ depending on how θ is chosen. The momentum operator will be self adjoint since 4.5 will be satisfied and since, given $f \in \mathbf{H}$,

$$\begin{aligned} (\hat{p} \pm i)g_\pm &= f \\ \Rightarrow \partial_x g_\pm \mp g_\pm &= if \end{aligned} \tag{4.13}$$

which has a solution

$$g_\pm = e^{\pm x}[g_0 + i\int_0^x f(x')e^{\mp x'}\,dx']. \tag{4.14}$$

The final requirement of 4.9 is that $g_\pm$ be in $\mathbf{D}(\hat{p})$. This can easily be seen to be the case if

$$\frac{g_\pm(1)}{g_\pm(0)} = e^{-i\theta} \tag{4.15}$$

so that

$$g_0 = ie^{i\theta\pm 1}\int_0^1 f(x')e^{\mp x'}\,dx'. \tag{4.16}$$

From 4.9 it follows that $\hat{p}$ is self adjoint.

If 4.8 had been taken as the definition of the momentum operator then 4.15 would become

$$g_\pm(0) = g_\pm(1) = 0$$

which leads to the statement

$$0 = g_\pm(1) = ie^{\pm 1}\int_0^1 f(x')e^{\mp x'}\,dx'$$

which cannot be true for *arbitrary* $f \in \mathbf{H}$. This is consistent with the earlier conclusion that 4.8 is not self adjoint.

The free particle Hamiltonian (taken elsewhere to be $\hat{p}^2/2$) is next to be defined. Let

$$\begin{aligned} \hat{\mathcal{H}} g(x) &= -\partial_x^2 g(x) \\ \text{where } g(0) &= g(1) = 0. \end{aligned} \tag{4.17}$$

The choice of boundary conditions is based on physical reasons and is not unique. $\hat{\mathcal{H}}$ is Hermitian:

$$\begin{aligned} \langle \hat{\mathcal{H}} f | g \rangle &= \int_0^1 (\hat{\mathcal{H}} f)^* g \, dx \\ &= -\partial_x f^* g|_0^1 + f^* \partial_x g|_0^1 + \langle f | \hat{\mathcal{H}} g \rangle \\ &= \langle f | \hat{\mathcal{H}} g \rangle. \end{aligned} \tag{4.18}$$

for all $f, g \in \mathbf{D}(\hat{\mathcal{H}})$. Further, from 4.9,

$$-\partial_x^2 g_\pm \pm i g_\pm = f,$$

where $f \in \mathbf{H}$, implies that

$$g_\pm = G_\pm [g_0 + \int_0^x \frac{g_1 - \int_0^{x'} G_\pm f(x'') \, dx''}{G_\pm^2} \, dx'] \tag{4.19}$$

where g_0 and g_1 are constants and $G_\pm$ are solutions of the homogeneous equation

$$-d_x^2 G_\pm \pm i G_\pm = 0.$$

The solution, 4.19, will be in $\mathbf{D}(\hat{\mathcal{H}})$ if

$$\begin{aligned} g_0 &= 0 \\ g_1 &= \frac{\int_0^1 \frac{\int_0^{x'} G_\pm f \, dx''}{G_\pm^2} \, dx'}{\int_0^1 G_\pm^{-2} \, dx} \end{aligned} \tag{4.20}$$

From this and 4.9 it follows that $\hat{\mathcal{H}}$ is self adjoint.

It is very important to realise that $\hat{\mathcal{H}}$, defined by 4.17 is *not* $\hat{p}^2$! The domain of $\hat{p}^2$ is a subspace of the domain of $\hat{p}$ which contains all the elements, g, for which $\hat{p}g \in \mathbf{D}(\hat{p})$, so that $\hat{p}^2 g = \hat{p}(\hat{p}g)$ is defined. In fact

$$\mathbf{D}(\hat{p}^2) = \{g | g(0) = e^{i\theta} g(1), \partial_x g(0) = e^{i\theta} \partial_x g(1)\}. \tag{4.21}$$

Defined this way, $\hat{p}^2$ is obviously Hermitian since 4.18 will be true and g_0 and g_1 can be found in a straightforward manner such that $g_\pm \in \mathbf{D}(\hat{p}^2)$. This process may be continued and higher powers of momentum may be defined. In a similar fashion, higher powers of the free particle Hamiltonian, $\hat{\mathcal{H}}$, may be defined. With this done, it is possible to define quantities like $e^{-i\hat{p}\Delta}$ in terms of their Taylor series (Here, Δ is a real number).

Now the domain of a quantity like $e^{-i\hat{p}\Delta}$ can easily be seen to be functions for which *all* derivatives satisfy the boundary conditions $f^{(n)}(0) = e^{i\theta} f^{(n)}(1)$ (where $f^{(n)}$ denotes the n^{th} derivative of f). This may seem like a restrictive domain, but it is, in fact, dense in the Hilbert space. Further, it is a bounded operator which may be extended to act on the entire Hilbert space by means of Cauchy sequences, as mentioned before: If f_n is a convergent sequence of functions in the domain of $e^{-i\hat{p}\Delta}$ with a limit point, f, outside of the domain, then $e^{-i\hat{p}\Delta} f$ may be defined as $lim_{n\to\infty} e^{-i\hat{p}\Delta} f_n$. The boundedness of the operator, $e^{-i\hat{p}\Delta}$, guarantees the convergence of the limit. In general, unbounded operators, such as the momentum operator, will diverge under such a limiting process.

There is nothing in the above discussion to determine θ (introduced in 4.12). The physical meaning of θ has been examined by Wightman [25] and Capri [24]. What is important is the effect that θ has on the translation operator:

$$\hat{T}(\Delta) \equiv e^{-i\hat{p}\Delta} \tag{4.22}$$

In unrestricted space, $\hat{T}$ is known [22] to translate a function by an amount Δ:

$$\hat{T}(\Delta)f(x) = f(x-\Delta). \tag{4.23}$$

However, on the interval $[0,1]$, the effect is somewhat different. The eigenfunctions of $\hat{p}$ are

$$\phi_n = e^{i(2n\pi-\theta)x} \tag{4.24}$$

with eigenvalues

$$p_n = 2n\pi - \theta \tag{4.25}$$

An arbitrary state, Ψ, can be expanded in terms of these eigenfunctions so that

$$\Psi = \sum_{n=-\infty}^{\infty} a_n e^{i(2n\pi-\theta)x}. \tag{4.26}$$

The eigenfunctions, ϕ_n are obviously in the domain of $\hat{T}(\Delta)$ so that $\hat{T}(\Delta)\Psi$ may be evaluated with 4.26:

$$\begin{aligned}
\hat{T}(\Delta)\Psi &= e^{-i\hat{p}\Delta}\Psi \\
&= \sum_{j=0}^{\infty}\frac{(-i\Delta)^j}{j!}\sum_{n=-\infty}^{\infty} a_n \hat{p}^n e^{i(2n\pi-\theta)x} \\
&= \sum_{n=-\infty}^{\infty} a_n e^{i(2n\pi-\theta)(x-\Delta)}.
\end{aligned} \tag{4.27}$$

It is tempting to write this as $\Psi(x-\Delta)$, but it must not be forgotten that $\Psi'(x) \equiv \Psi(x-\Delta)$ is only defined for $0 < x-\Delta < 1$ and not $0 < x < 1$, so that $\Psi'(x)$ is not a well defined function on the interval $[0,1]$. A closer look at 4.27 reveals that the effect of $\hat{T}(\Delta)$ is to shift the function to the right by an amount Δ, and return the portion that leaves $[0,1]$ via the opposite wall with a phase shift of $e^{i\theta}$. A commonly used term describing this is 'physics on a circle', which implies that, in some sense the variable, x, is an angle-like variable.

It is now becoming clear why it is undesirable to define $\hat{\mathcal{H}}$ in terms of the momentum operator: $\hat{p}^2$ will not generate the reflection needed at the boundaries to

simulate a box with rigid walls. The free particle Hamiltonian, on the other hand, will generate the desired behaviour. The operator $\hat{\mathcal{H}}$ has eigenstates

$$\phi_n = \sqrt{2}\sin(n\pi x) \tag{4.28}$$

which form a complete basis set, so that an arbitrary wavefunction can be expanded:

$$\Psi(x, t=0) = \sum_{n=1}^{\infty} a_n \sqrt{2}\sin(n\pi x). \tag{4.29}$$

The time evolution operator associated with $\hat{\mathcal{H}}$ is

$$\hat{U} = e^{-i\hat{\mathcal{H}}t/2}. \tag{4.30}$$

The wavefunction, Ψ given by 4.29, is in the domain of $\hat{U}$ so that $\hat{U}\Psi$ can be evaluated. Notice that Ψ, given by 4.26, is *not* in the domain of $\hat{U}$.

$$\begin{aligned} \Psi(x,t) &= e^{-i\hat{\mathcal{H}}t/2} \sum_{n=1}^{\infty} a_n \sqrt{2}\sin(n\pi x) \\ &= \sum_{n=1}^{\infty} a_n \sqrt{2}\sin(n\pi x) e^{-i(n\pi)^2 t/2}. \end{aligned} \tag{4.31}$$

The wall reflection can easily be seen from the behaviour of a wavepacket made up of the first two eigenstates:

$$\Psi(x,t) = e^{-i\pi^2 t/2}\sin(\pi x) + e^{-i(2\pi)^2 t/2}\sin(2\pi x), \tag{4.32}$$

for which $\langle \hat{p} \rangle$ is

$$\langle \hat{p} \rangle = 8/3 \sin[3\pi^2 t/2]. \tag{4.33}$$

This can be compared with the behaviour of a wavefunction whose generator of motion is

$$\hat{U} = e^{-i\hat{p}^2 t/2}. \tag{4.34}$$

A wavefunction constructed from the first two positive eigenstates of $\hat{p}^2$ is:

$$\Psi = (1/\sqrt{2})[e^{i[(2\pi-\theta)x-(2\pi-\theta)^2 t/2]} + e^{i[(4\pi-\theta)x-(4\pi-\theta)^2 t/2]}] \tag{4.35}$$

for which $\langle \hat{p} \rangle$ is

$$\langle p \rangle = 1/2[(2\pi - \theta) + (4\pi - \theta)]. \tag{4.36}$$

As is evident, there is no change in the sign of the momentum and the wavepacket is transmitted through the right hand wall of the box (at $x = 1$) with a constant momentum. As was discussed earlier, probability is conserved as the portion of the wavepacket which leaves, reappears through the left hand wall (at $x = 0$). It is apparent that the different domains for $\hat{p}^2$ and $\hat{\mathcal{H}}$ determine which series expansions can be used to represent a wavefunction. It is the difference in these basis sets which produces the different behaviour of the two cases.

The point of the previous example is to demonstrate how crucial the choice of operator is when trying to represent the physical behaviour of the system, and to motivate the choice of $\hat{\mathcal{H}}$ for the free particle generator of motion. This discussion also gives a clue as to what the source of the discrepancy between the Schrödinger and Heisenberg approaches, discussed in the previous chapter, could be. Recall that the Heisenberg equations of motion were given in 3.29 and 3.30 as

$$\begin{aligned} i\hbar\, d_\tau \hat{x} &= [\hat{x}, \hat{H}], \\ i\hbar\, d_\tau \hat{p} &= [\hat{p}, \hat{H}], \end{aligned} \tag{4.37}$$

where $\hat{H}$ was given by 3.31, and will now be correctly written as

$$\hat{H} = \hat{\mathcal{H}}/2m + mg(\tau)\hat{x}^2/2. \tag{4.38}$$

For the remainder of this chapter and for chapter 6, operators will be *assumed* to be Heisenberg operators (with an implied time dependence) unless otherwise denoted with a subscript 0. Occasionally the time dependence of an operator will be indicated for emphasis.

To solve these equations it is necessary to evaluate the commutators $[\hat{x}, \hat{\mathcal{H}}]$, $[\hat{p}, \hat{\mathcal{H}}]$ and $[\hat{p}, \hat{x}^2]$. This will be done by first evaluating the commutators at $\tau =$

0—$[\hat{x}_0, \hat{\mathcal{H}}_0]$, $[\hat{p}_0, \hat{\mathcal{H}}_0]$ and $[\hat{p}_0, \hat{x}_0^2]$—and then noting the general relationship: If, for Heisenberg operators $\hat{A}$,$\hat{B}$ and $\hat{C}$

$$[\hat{A}_0, \hat{B}_0] = \hat{C}_0,$$

then

$$[\hat{A}(\tau), \hat{B}(\tau)] = \hat{C}(\tau).$$

As was discussed earlier, particular attention must be paid to defining the operator combinations which appear in these commutators. The operators are dealt with in order:

1. The first commutator is

$$[\hat{x}_0, \hat{\mathcal{H}}_0] = [\hat{x}_0\hat{\mathcal{H}}_0 - \hat{\mathcal{H}}_0\hat{x}_0], \tag{4.39}$$

which has in its domain all functions, f, such that the combinations $\hat{x}_0\hat{\mathcal{H}}_0$ and $\hat{\mathcal{H}}_0\hat{x}_0$ are defined.

$$\begin{aligned} \mathbf{D}([\hat{x}_0, \hat{\mathcal{H}}_0]) &= \{f | f \in \mathbf{D}(\hat{\mathcal{H}}_0), f \in \mathbf{D}(\hat{x}_0), \hat{\mathcal{H}}_0 f \in \mathbf{D}(\hat{x}_0), \hat{x}_0 f \in \mathbf{D}(\hat{\mathcal{H}}_0)\} \\ &= \{f | f(0) = f(1) = 0\} \end{aligned} \tag{4.40}$$

For functions in $\mathbf{D}([\hat{x}_0, \hat{\mathcal{H}}_0])$,

$$[\hat{x}_0, \hat{\mathcal{H}}_0] = 2i\hbar\hat{\mathcal{P}}_0, \tag{4.41}$$

where $\hat{\mathcal{P}}_0$ is defined by 4.8. It should be recalled that in unrestricted space the commutator is

$$[\hat{x}_0, \hat{\mathcal{H}}_0] = 2i\hbar\hat{p}_0. \tag{4.42}$$

The two commutators, 4.41 and 4.42, differ because of the size of the domains of $\hat{p}_0$ and $\hat{\mathcal{P}}_0$. The domain of $\hat{\mathcal{P}}_0$ can be extended by the method described before; Cauchy sequences which converge outside of the domain of the operator

may be used to extend the domain of the operator. An operator, defined over its extended domain, is called the *closure* of the operator and is denoted with an overbar. An operator will only be distinguished from its closure if there is a possibility of confusion. Since $\hat{\mathcal{P}}_0$ is an unbounded operator, $\overline{\mathcal{P}}_0$ is expected to contain divergent terms. However, provided the divergences are weak, they will not pose insurmountable problems. Let $f \in \mathbf{D}(\hat{p}_0)$ be given, and write it as

$$\begin{aligned} f &= a + bx + g(x), \\ a &= f(0), \\ b &= f(1) - f(0) \\ g(x) &\in \mathbf{D}(\hat{\mathcal{P}}_0) \end{aligned} \tag{4.43}$$

Now the Cauchy sequence

$$f_N = \sum_{n=1}^{N} (2/n\pi)[a - (a+b)(-1)^n] \sin(n\pi x) + g(x) \tag{4.44}$$

can be defined. The sequence converges in the norm to $f \in \mathbf{D}(\overline{\mathcal{P}}_0)$, but each of the terms, f_N, is in $\mathbf{D}(\hat{\mathcal{P}}_0)$. Then it is possible to define

$$\begin{aligned} \overline{\mathcal{P}}_0 f &\equiv \lim_{N\to\infty} \hat{\mathcal{P}}_0 f_N \\ &= -i\hbar \lim_{N\to\infty} \sum_{n=1}^{N} 2[a - (a+b)(-1)^n] \cos(n\pi x) + -i\hbar\partial_x g(x) \\ &= -i\hbar[\partial_x f + 2f(0)\delta(x) - 2f(1)\delta(1-x)] \end{aligned} \tag{4.45}$$

For the moment, it is assumed that the divergences can be dealt with as necessary, and $\hat{\mathcal{P}}_0$ will now be extended:

$$\begin{aligned} \overline{\mathcal{P}}_0 &= \hat{p}_0 - 2i\hbar[\delta(\hat{x}_0) - \delta(\hat{I} - \hat{x}_0)], \\ \mathbf{D}(\overline{\mathcal{P}}_0) &= \mathbf{D}(\hat{p}_0). \end{aligned} \tag{4.46}$$

The identity operator is denoted by $\hat{I}$. At any time, then, the following hold true

$$[\hat{x}, \hat{\mathcal{H}}] = 2i\hbar\hat{\mathcal{P}} \tag{4.47}$$

$$\begin{aligned}\overline{[\hat{x},\hat{\mathcal{H}}]} &= 2i\hbar\overline{\mathcal{P}} \\ &= 2i\hbar\hat{p} + 4\hbar^2[\delta(\hat{x}) - \delta(\hat{I} - \hat{x})]. \end{aligned} \tag{4.48}$$

It is clear, from 4.46 that $\overline{\mathcal{P}}$ is similar to $\hat{p}$, but differs by a term which is not Hermitian (an imaginary function of x is, in fact, anti–Hermitian).

2. The second commutator to be dealt with is $[\hat{p}_0, \hat{\mathcal{H}}_0]$. From the form of $[\hat{p}_0, \hat{\mathcal{H}}_0]$ it follows that

$$\mathbf{D}([\hat{p}_0, \hat{\mathcal{H}}_0]) = \{f | f(0) = f(1) = 0, \partial_x f\Big|_0 = \partial_x f\Big|_1 = 0,\ \partial_x^2 f\Big|_0 = e^{i\theta}\partial_x^2 f\Big|_1\}. \tag{4.49}$$

For elements in $[\hat{p}_0, \hat{\mathcal{H}}_0]$,

$$\begin{aligned}[\hat{p}_0, \hat{\mathcal{H}}_0]f &= i\hbar^3\partial_x^3 f - i\hbar^3\partial_x^3 f \\ &= 0. \end{aligned} \tag{4.50}$$

The operator, $[\hat{p}_0, \hat{\mathcal{H}}_0]$, may be extended by the same method used above and, since it is a bounded operator, it may be extended to the entire Hilbert space. Then, for any value of τ,

$$\begin{aligned}\overline{[\hat{p}, \hat{\mathcal{H}}]} &= 0 \\ \mathbf{D}(\overline{[\hat{p}, \hat{\mathcal{H}}]}) &= \mathbf{H}. \end{aligned} \tag{4.51}$$

By a similar calculation

$$\begin{aligned}\overline{[\hat{\mathcal{P}}, \hat{\mathcal{H}}]} &= 0 \\ \mathbf{D}(\overline{[\hat{\mathcal{P}}, \hat{\mathcal{H}}]}) &= \mathbf{H}. \end{aligned} \tag{4.52}$$

3. The third commutator is $[\hat{p}_0, \hat{x}_0^2]$. It has a domain

$$\mathbf{D}([\hat{p}_0, \hat{x}_0^2]) = \{f | f(0) = f(1) = 0\}, \tag{4.53}$$

and for elements in this domain

$$[\hat{p}_0, \hat{x}_0^2]f = -2i\hbar x f. \tag{4.54}$$

Now $\hat{x}_0$ is a bounded operator and may therefore be extended to have the entire Hilbert space in its domain. Again,

$$\begin{aligned} [\hat{p}, \hat{x}^2] &= -2i\hbar\hat{x} \\ \mathbf{D}([\hat{p}, \hat{x}^2]) &= \mathbf{H} \end{aligned} \tag{4.55}$$

and

$$\begin{aligned} [\hat{\mathcal{P}}, \hat{x}^2] &= -2i\hbar\hat{x} \\ \mathbf{D}([\hat{\mathcal{P}}, \hat{x}^2]) &= \mathbf{H} \end{aligned} \tag{4.56}$$

In general,

$$\begin{aligned} [\hat{p}, \hat{x}^N] = -i\hbar N\hat{x}^{N-1} \quad [\hat{\mathcal{P}}, \hat{x}^N] = -i\hbar N\hat{x}^{N-1} \\ [\hat{x}, \hat{p}^N] = i\hbar N\hat{p}^{N-1} \quad [\hat{x}, \hat{\mathcal{P}}^N] = i\hbar N\hat{\mathcal{P}}^{N-1} \end{aligned} \tag{4.57}$$

follow from the identity (for operators $\hat{A}, \hat{B}$)

$$[\hat{A}, \hat{B}^n] = [\hat{A}, \hat{B}]\hat{B}^{n-1} + \hat{B}[\hat{A}, \hat{B}]\hat{B}^{n-2} + \ldots + \hat{B}^{n-1}[\hat{A}, \hat{B}], \tag{4.58}$$

and the commutators, $[\hat{x}, \hat{p}] = [\hat{x}, \hat{\mathcal{P}}] = i\hbar$.

The Heisenberg equations, 3.29 and 3.30, become

$$\begin{aligned} d_\tau\hat{x} &= (-i/\hbar)\{[\hat{x}, \hat{\mathcal{H}}/2m] + [\hat{x}, mg(\tau)\hat{x}^2/2]\} \\ &= \hat{\mathcal{P}}/m, \end{aligned} \tag{4.59}$$

$$\begin{aligned} d_\tau\hat{\mathcal{P}} &= (-i/\hbar)\{[\hat{\mathcal{P}}, \hat{\mathcal{H}}/2m] + [\hat{\mathcal{P}}, mg(\tau)\hat{x}^2/2]\} \\ &= -mg(\tau)\hat{x} \end{aligned} \tag{4.60}$$

and

$$\begin{aligned} d_\tau \hat{p} &= (-i/\hbar)\{[\hat{p}, \hat{\mathcal{H}}/2m] + [\hat{p}, mg(\tau)\hat{x}^2/2]\} \\ &= -mg(\tau)\hat{x}. \end{aligned} \tag{4.61}$$

Equation 4.59 gives a definition of $\hat{\mathcal{P}}(\tau)$. It will be shown in chapter 6 that this definition agrees with the definition given in 4.8 at $\tau = 0$. Equations 4.60 and 4.61 are equations of motion for the two operators, $\hat{\mathcal{P}}(\tau)$ and $\hat{p}(\tau)$. The identical form of 4.60 and 4.61 hide the very different behaviour which they generate for the two operators. It will be shown in chapter 6 that the difference in the domains allows the effects of the walls to be included in $\hat{\mathcal{P}}(\tau)$, but not in $\hat{p}(\tau)$. This is not surprising; it was shown in equations 4.30–4.36 that the boundary conditions have a tremendous impact on the evolution of the system.

For now it will be shown that, in the special case $g(\tau) = 0$, the two most obvious solutions for 4.59 are wrong. The first choice is

$$\hat{x} = \hat{p}_0 \tau/m + \hat{x}_0, \tag{4.62}$$

for which

$$d_\tau \hat{x} = \hat{p}_0/m. \tag{4.63}$$

Combining 4.59 and 4.60 gives

$$d_\tau \hat{x} = \hat{\mathcal{P}}_0/m, \tag{4.64}$$

which disagrees with 4.63. Further, the discrepancy between 4.63 and 4.64 is not just that the domains are different. Taking the closure of 4.63 gives the condition

$$\overline{d_\tau \hat{x}} = \hat{p}_0 - i\hbar[\delta(\hat{x}) - \delta(\hat{I} - \hat{x})], \tag{4.65}$$

which is still wrong. The second obvious choice for $\hat{x}$ is

$$\hat{x} = \hat{\mathcal{P}}_0 \tau/m + \hat{x}_0. \tag{4.66}$$

It satisfies the Heisenberg equations of motion but fails because it is not self adjoint (since $\hat{\mathcal{P}}_0$ is not self adjoint). Self adjointness guarantees the existence of a complete set of eigenfunctions with real eigenvalues. It is easily seen that $\hat{x}$, given by 4.66 has no real eigenvalues. If

$$\hat{x}\phi = \kappa\phi,$$

where κ is an eigenvalue and ϕ is an eigenfunction, then

$$\phi = e^{-im[x^2/2-\kappa x]/(\hbar\tau)}.$$

There are no real values of κ for which ϕ will vanish at the boundaries. This lack of eigenfunctions is one of the major difficulties in working with the solution which is presented in chapter 6.

This chapter is concluded with a brief discussion of momentum. Obviously $\hat{\mathcal{P}}$ and $\overline{\mathcal{P}}$ are not suitable to represent the observable momentum; neither is self adjoint. Unfortunately, the only remaining candidate, $\hat{p}$ also fails to be suitable. In the special case $g(\tau) = 0$, for example, equation 4.61 implies that $\langle\hat{p}\rangle$ is a conserved quantity for any Heisenberg wavefunction. This is the same result that is found in equations 4.34—4.36, where the behaviour of $\langle\hat{p}\rangle$ is examined in the Schrödinger picture. This kind of behaviour is not characteristic of the mechanical momentum which is observed. To what does $\hat{p}$ correspond, then? In the classical Hamiltonian

$$H = p^2/2m,$$

the quantity, p, is a conserved quantity, while the mechanical (observed) momentum is $\pm p$. The operator, $\hat{p}$, then corresponds to the *canonical* momentum.

Chapter 5

The Semiclassical Limit

Correspondence between the classical and quantum Fermi–Ulam Accelerator is not an obvious thing. There are a number of technical problems, specific to this particular model, as well as a number of problems which are generally present in the semiclassical limit of any system. Semiclassical physics is primarily a tool used for finding quantum mechanical information based on quasiclassical arguments. Traditionally, the question of finding classical information from a quantum system has not been as popular, mainly because classical mechanics is the simplest practical method of finding an answer in the classical domain. The problem of the transition from quantum to classical mechanics has often been relegated to the status of a philosophical problem, or explained in terms of statistical arguments. With the advent of experimentally realised single particle quantum systems (e.g. [9, 10]) the problem is becoming relevant and in need of an answer.

This chapter is not intended as a discussion of all aspects of semiclassical physics, but instead is meant as a review of some of the work specifically dealing with the semiclassical limit of the Fermi–Ulam Accelerator, and as a discussion of the differences in the classical and quantum treatments of the problem. This chapter will not answer the question of how classical behaviour (ie. a localised particle obeying classical equations of motion) can be found, in some limit, from quantum mechanics. It *will*, however, show how the information required to define the classical system is contained in the quantum system.

In order to compare the work of chapters 2 and 3, the treatments should be

made as similar as possible. The first step is to find a classical coordinate transformation analogous to 3.5 and 3.6. Such a transformation is given by the generating function (see [26, chapter 9], [19])

$$F_2 = \frac{xP}{L(t)} + \frac{mx^2\dot{L}}{2L} \tag{5.1}$$

which transforms the old coordinates

$$(x,p), \text{ where } 0 < x < L(t)$$

to the new coordinates

$$(X,P), \text{ where } 0 < X < 1 \tag{5.2}$$

according to

$$\begin{aligned} X &= \partial_P F_2 \\ &= x/L(t) \qquad (5.3) \\ p &= \partial_x F_2 \\ &= P/L(t) + mx\dot{L}(t)/L(t) \\ &= P/L(t) + mX\dot{L}(t). \qquad (5.4) \end{aligned}$$

The Hamiltonian will, for the moment, be taken as

$$H = \frac{p^2}{2m} + V(\frac{x}{L(t)}) \tag{5.5}$$

with V(x/L(t)) representing the moving walls of the box. This Hamiltonian transforms to

$$\begin{aligned} K &= H(x(X,P),p(X,P),t) + \partial_t F_2(x(X,P),P,t) \\ &= \frac{P^2}{2mL(t)^2} + \frac{1}{2}mL(t)\ddot{L}(t)X^2 + V(X). \qquad (5.6) \end{aligned}$$

The new Hamiltonian generates the equations of motion

$$\dot{X} = \frac{P}{mL^2} \tag{5.7}$$

$$\dot{P} = -mXL\ddot{L} - \partial_X V \tag{5.8}$$

The equations of motion for x and p generated by H can be regained by direct substitution. A rescaling of time, given by 3.16, will turn these into

$$\partial_\tau X = P \tag{5.9}$$

$$\partial_\tau^2 X + g(\tau)X + \frac{L^2(\tau)}{m}\partial_X V = 0. \tag{5.10}$$

The assumption is made that the potential representing the walls of the box is only felt by the particle for short periods of time, during the bounce. Near the wall of the box, the walls dominate the behaviour:

$$\partial_\tau^2 X + \frac{L^2(\tau)}{m}\partial_X V = 0.$$

The interaction is short enough that $L(\tau)$ is constant and this equation may be integrated once to give

$$\frac{1}{2}\left(\partial_\tau X\right)^2\Big|_b^a = \frac{L^2(\tau)}{m}\, V(X)\Big|_b^a$$

The limits of integration are chosen to be points just before (b) and after (a) the collision. At these points, V will rapidly become negligible and this becomes

$$P^2\Big|_b = P^2\Big|_a \tag{5.11}$$

In other words, the potential can be replaced with boundary conditions which change the sign of P at the turning points $X = 0$ and $X = 1$. Direct substitution for P and X will give back the boundary conditions given in chapter 2.

Away from the walls the potential, V, is negligible, so that the equation of motion for X becomes

$$\partial_\tau^2 X + g(\tau)X = 0. \tag{5.12}$$

From this it is possible to replace the Hamiltonian 5.6 with

$$\begin{aligned} K' &= L^2(\tau)K(t(\tau)) \\ &= \frac{P^2}{2m} + \frac{1}{2}mg(\tau)X^2 \end{aligned} \tag{5.13}$$

and the boundary conditions 5.11. There is, then, a set of canonical transformations which is analogous to the quantum transformations of chapter 3.

The comparison of the quantum and classical systems can now be carried out in the transformed coordinate system. There remains, however the question of how to compare them. The JWKB approximation [22, 27] is one of the most common semiclassical techniques. It is only useful in systems with time independent potentials (for which the classical action is separable), and so limits the discussion to the special form for L(t) given by 3.27. The form of the wavefunction in the JWKB approximation is

$$\Psi \sim \frac{e^{iS(X,\tau)/\hbar}}{\sqrt{\partial_X S(X,\tau)}} \tag{5.14}$$

where S is the classical action. The appeal of the JWKB approach is that it allows a direct comparison of a classical quantity, S, with a quantum quantity, Ψ. Unfortunately, a simple physical interpretation of the meaning of this is not obvious.

The standard approach to finding 5.14 is to start by finding the classical action. For a one dimensional Hamiltonian of the form

$$H = \frac{P^2}{2m} + U(X), \tag{5.15}$$

where U is the time independent potential, the Hamilton–Jacobi equation is

$$\frac{(\partial_X S)^2}{2m} + U(X) = -\partial_\tau S \tag{5.16}$$

implying that

$$S = \pm \int^X \sqrt{2m(E - U(X))}\, dx - E\tau, \tag{5.17}$$

where E is a separation constant. The momentum of the particle is given by

$$\begin{aligned} P &= \partial_X S \\ &= \pm\sqrt{2m(E - U(X))}. \end{aligned} \tag{5.18}$$

Thus the branch of 5.17 is determined by the sign of the momentum of the particle. As a result, the particle will change branches at the turning points of its trajectory. With the condition that S must be a continuous function along the trajectory, and the fact that S is always increasing along the trajectory, 5.17 turns out to have an infinite number of branches of either sign, distinguished by additive constants. If the turning points are at $X = 0$ and $X = 1$ then the n^{th} branch of the action will be

$$S_n = (-1)^n \int_0^X \sqrt{2m(E - U(X))}\, dX + \left\{ \begin{array}{l} n\Delta S \text{ if } n \text{ is even} \\ (n+1)\Delta S \text{ if } n \text{ is odd} \end{array} \right\} - E\tau. \quad (5.19)$$

where

$$\Delta S \equiv \int_0^1 \sqrt{2m(E - U(X))}\, dX$$

The particle can only be associated with one branch of the action at any given time, and therefore it will have an action of the form

$$S(X, \tau) = \sum_{n=-\infty}^{\infty} S_n \theta(\tau - \tau_n)\theta(\tau_{n+1} - \tau) \quad (5.20)$$

where $\theta(\tau)$ is the step function and the τ_n are the times at which the particle makes the n^{th} bounce from either the left or right turning points (this series is different from that defined in chapter 2 where only bounces from the moving wall are included). It should be observed that the most important effect of the boundaries is to determine a sequence of turning times (the quantity ΔS follows from a knowledge of turning times if dX is replaced with $d_\tau X\, d\tau$ and the integration is performed with respect to τ), and that the general form of S is independent of these times.

Equation 5.20 describes the motion of a particle as a sequence of scatterings from the walls of the box. In the JWKB approximation the final wavefunction is considered as a sum of scattered and re-scattered waves. Such a wavefunction will not depend on a series of scattering times, and yet this information must be contained in the quantum wavefunction (otherwise the classical system could not be a limiting case of the quantum system). The aim of the next few pages is to show how the

information required to define the classical problem is contained within the quantum solution.

The JWKB wavefunction, 5.14, is an approximate solution to a Schrödinger equation of the form

$$-\frac{\hbar^2}{2m}\partial_X^2\Psi + U(X)\Psi = i\hbar\partial_\tau\Psi. \tag{5.21}$$

When substituted in, the approximation turns the wave equation into

$$\begin{aligned} i\hbar\partial_\tau(\partial_X S)^{-1/2} - (\partial_X S)^{-1/2}\partial_\tau S &= -\frac{\hbar^2}{2m}[\partial_X^2(\partial_X S)^{-1/2} - (1/\hbar)^2(\partial_X S)^{-1/2}(\partial_X S)^2] \\ &\quad + U(X)(\partial_X S)^{-1/2}. \end{aligned}$$

Choosing S to be the classical action given by 5.16 simplifies this to

$$\hbar^2\partial_X^2(\partial_X S)^{-1/2} = 0, \tag{5.22}$$

which is obviously not generally true. The value of 5.14 as an approximation, then, depends on 5.22 being approximately true. The requirement of the relative smallness of the left hand side of 5.22 can be rewritten

$$\hbar^2\sqrt{P}\partial_X^2 P^{-1/2} \ll P^2. \tag{5.23}$$

This condition will be met in regions in which the potential is relatively constant, and in regions in which there are no classical turning points. For a quadratic potential embedded in a box, this will be true at large energies everywhere except at the edges of the box. A different approximation needs to be made near the edge of the box.

The standard approach near a boundary [27] is to take a Fourier transform of 5.21 , solve a similar approximation to the one above, and Fourier transform back to the position space. This approach requires that the boundary be soft enough that the region of validity of the approximation be several wavelengths. Unfortunately, this will not be the case in a box, where the assumption is that the wall appears hard for all energies of the wavefunction.

The use of the solution for the wavefunction near the boundaries is to give a condition for joining incident and scattered waves at the boundary. The condition takes the form of a phase shift between the waves. The complete solution to 5.21 is formed of an infinite sum of incident and scattered waves, joined by these phase shifts:

$$\Psi = \sum_{n=-\infty}^{\infty} \frac{e^{i(S_n/\hbar+\phi_n)}}{\sqrt{\partial_X S_n}}, \tag{5.24}$$

where ϕ_n are the phase shifts and are closely related to the Maslov indices. In 5.24, the $(n+1)^{th}$ term is the scattered wave due to the n^{th} term, and S_n is given by 5.19. This kind of series is similar to the Bremmer series for multiply reflected waves, discussed in [28]. By choosing the phase shifts, $\phi_n = -n\pi/2$, which result from the standard fashion of dealing with the boundaries, 5.24 becomes

$$\begin{aligned}\Psi &= \left\{ \frac{e^{(i/\hbar)\int_0^X \sqrt{2m(E-U(X'))}\,dX'} \pm e^{(-i/\hbar)\int_0^X \sqrt{2m(E-U(X'))}\,dX'}}{[2m(E-U(X))]^{1/4}} \right\} e^{-iE\tau/\hbar} \\ &\times \sum_{n=-\infty}^{\infty} e^{in[2/\hbar\int_0^1 \sqrt{2m(E-U(X'))}\,dX' - \pi]}.\end{aligned} \tag{5.25}$$

The infinite sum is a delta–function and will only be nonzero for

$$\begin{aligned}\Delta S &= \int_0^1 \sqrt{2m(E-U(X'))}\,dX' \\ &= \hbar\pi[k+1/2],\end{aligned} \tag{5.26}$$

where k is an integer. The physical meaning of 5.25 is that the infinite sum of scattered waves will only interfere constructively for certain, special values of E. The quantisation rule, 5.26, applies to any one dimensional, time independent system, and should be compared with the Bohr–Sommerfeld (BS) quantisation rule [29]:

$$\Delta S = \hbar k\pi \tag{5.27}$$

The JWKB quantisation rule will give wavefunctions which do not vanish at both ends of the interval $[0,1]$ and gives energy eigenvalues which never converge to the

true eigenvalues in the large energy limit. BS quantisation converges to the true energy eigenvalues in the large energy limit and gives wavefunctions which vanish at both ends of the interval. On the other hand, in a harmonic oscillator potential, JWKB quantisation gives accurate results where BS quantisation fails.

The effect of the boundary conditions in 5.25 is to set the energy eigenstates; the actual form of the wavefunction does not explicitly depend on the boundaries. This is reminiscent of what was said about the classical system—that the turning times are determined by the boundaries while the form of the solution is independent of the boundaries. The connection between the form of the wavefunction and the form of the classical solution is obvious and is given by equation 5.14. What will be shown now, through an explicit example, is how the classical turning times for the Fermi–Ulam Accelerator are contained in the quantisation of the energy.

If the Hamiltonian,

$$H = \frac{P^2}{2m} + \frac{mg_0X^2}{2}, \tag{5.28}$$

where g_0 is constant, is embedded in a box with walls at $X = 0$ and at $X = 1$, then the semiclassical wavefunction will be

$$\begin{aligned} \Psi_n &= \left\{ \frac{e^{iS_0(X,n)/\hbar} \pm e^{-iS_0(X,n)/\hbar}}{[2m(E_n - mg_0X^2/2)]^{1/4}} \right\} e^{-iE_nt/\hbar} \\ S_0(X,n) &= \frac{E_n}{\sqrt{g_0}} \arcsin(\sqrt{\frac{mg_0}{2E_n}}X) + \sqrt{\frac{mE_n}{2}}\, X\sqrt{1 - \frac{mg_0X^2}{2E_n}}. \end{aligned} \tag{5.29}$$

The eigenvalues, E_n, are determined in the large energy limit by a perturbation expansion over g_0. The large energy limit should not be confused with a classical limit, which will be described shortly. The large energy limit is a computational convenience. To first order in g_0,

$$E_n \sim \frac{(\hbar n\pi)^2}{2m} + mg_0[\frac{1}{6} - \frac{1}{(2n\pi)^2}] \tag{5.30}$$

The goal, now, is to show how the spectrum, E_n, can be compared with the

JWKB or BS semiclassical spectrum (given by 5.26 and 5.27) to give both the classical turning points (which, in this case, are $X = 0$ and $X = 1$) and the classical turning times. Substituting 5.30 into the explicit form for S_0 given in 5.29 and carrying terms to order $g_0/n\pi$ gives

$$\Delta S(X,n) \sim \hbar n\pi(b-a) + \frac{m^2 g_0}{6\hbar n\pi}[b-a-(b^3-a^3)]. \tag{5.31}$$

Here, b and a are the unknown turning points. They will, in general depend on n. The classical limit is taken as follows: A region is found in which the eigenstates, E_n, are dense enough that $\delta_n a \sim \delta_n b \sim 0$, and in which any classical energy may be approximated well by a specific quantum eigenstate. The term $\delta_n a$ is defined as $a(n+1) - a(n)$.

For a box, whose turning points are fixed, the semiclassical limit implies only that the eigenvalues $E_n = (\hbar n\pi)^2/(2mL^2)$ (where L is the width of the box) become closely spaced. The classical limit, for a box then, is that the spacing of the walls, L becomes large relative to the eigenvalue , n. In this case, the classical limit is clearly *not* the large energy limit. For a harmonic oscillator, for which $E_n = \hbar\,\omega\,[n + 1/2]$ (ω^2 is the oscillator strength), the turning points are at $\pm\sqrt{\hbar[2n+1]/(m\omega)}$. Then $\delta_n\sqrt{\hbar[2n+1]/(m\omega)} \sim \sqrt{\hbar/([n+1/2]m\omega)}$ which becomes small in the large–n limit. The eigenstates will be closely spaced if the oscillator strength is moderate. For the harmonic oscillator, the large energy limit corresponds to the semiclassical limit.

For equation 5.31, the semiclassical limit implies that

$$\delta_n\Delta S(X,n) \sim \hbar\pi(b-a) - \frac{m^2 g_0}{6\hbar n^2\pi}[b-a-(b^3-a^3)]. \tag{5.32}$$

But, for either the JWKB or BS quantisation

$$\delta_n\Delta S(X,n) = \hbar\pi$$

so that

$$1 \sim (b-a) - \frac{m^2 g_0}{6(\hbar n\pi)^2}[b-a-(b^3-a^3)]. \tag{5.33}$$

The statement that 5.33 must be independent of n immediately yields the turning points $b = 1, a = 0$ or $b = 0, a = -1$. These solutions are in fact the same solution under a coordinate reflection. It is not necessary to find 5.33 to find the turning times, however. Instead, the classical equation of motion generated by the classical action is [26, chapter 10]:

$$\beta = \partial_E S_0 - \tau, \tag{5.34}$$

where β is a constant of the motion. With 5.29, this becomes

$$\tau + \beta = g_0^{-1/2} \arcsin(\sqrt{\frac{mg_0}{2E}} X)$$

and the time between turning points is

$$\Delta\tau = g_0^{-1/2}(\arcsin(\sqrt{\frac{mg_0}{2E}} b) - \arcsin(\sqrt{\frac{mg_0}{2E}} a)). \tag{5.35}$$

Here, E is the classical constant of motion and should not be confused with E_n, the quantised eigenvalues. Write

$$E \equiv \frac{(\hbar z \pi)^2}{2m} + mg_0[\frac{1}{6} - \frac{1}{(2z\pi)^2}], \tag{5.36}$$

where z is a continuous parameter. Then 5.35 can be written approximately as

$$\Delta\tau \sim \frac{m(b-a)}{\hbar z \pi} + \frac{m^3 g_0}{6(\hbar z \pi)^3}[(b^3 - a^3) - (b - a)]. \tag{5.37}$$

The requirements of the semiclassical regime are that it be possible to approximate z by the nearest n in value. From 5.37 and 5.33 it follows that

$$\begin{aligned} \Delta\tau &\sim \frac{m}{n\hbar^2\pi^2}\delta_n \Delta S_0 \\ &\sim \frac{m}{\hbar n \pi} \\ &\sim \sqrt{\frac{m}{2E}} + \frac{g_0}{6}(\frac{m}{2E})^{3/2}. \end{aligned} \tag{5.38}$$

Simple inspection reveals that the first equation is true for any value of g_0 provided the system is in the semiclassical domain, while the third equation is the explicit

solution for the case mg_0/E is small. The results in 5.38 agree to first order in g_0 with the solution obtained by setting $b = 1, a = 0$ in 5.35.

The above results can be summarised: If, from the wavefunction, it is possible to find the classical action, then the classical equations of motion will follow (equation 5.34). In the semiclassical regime, defined in terms of the density of eigenstates, the turning points and turning times can also be found directly from the energy spectrum and either of the semiclassical quantisation rules (equation 5.38). The results can be generalised to include any time independent potential in the semiclassical regime:

$$\Delta\tau \sim \frac{\delta_n \Delta S_0}{\delta_n E_n}. \tag{5.39}$$

This result supports the idea that classical behaviour is a property of groups of closely spaced quantum eigenstates. There has been some discussion [7] about whether classical mechanics depends on the behaviour of single eigenstates or groups of eigenstates. The most interesting feature of equation 5.39 is that the chaotic behaviour of the classical system manifests itself in the sequence of turning times, t_n (recall the equations 3.1 and 3.2). Equation 5.39 provides a direct method of formulating a condition for classical stochasticity in terms of the quantum eigenstates in the special case for which the wall motion is given by 3.27 (ie. $g(\tau)$ is piecewise constant).

Although it has been shown that the information required to define the classical problem is contained within the quantum wavefunction, nothing has been said about the way the classical behaviour comes about in the semiclassical limit. This is not a trivial problem. The usual way to produce a classical limit is to construct localised wavepackets which represent the classical particle. The behaviour of the wavepacket is given by Ehrenfest's theorem (see, for example [22]), which states that for *any* wavepacket

$$d_\tau^2 \langle \hat{x} \rangle = -\langle \partial_x V(x) \rangle. \tag{5.40}$$

This is similar to the classical equation of motion for a particle, except that the partial

derivative appears *inside* the expectation value brackets. For a localised wavepacket, centred at x_0,

$$\begin{aligned}\langle \partial_x \hat{V}(x) \rangle &= \int \psi^* \partial_x \hat{V}(x) \psi \, dx \\ &\sim \partial_{x_0} V(x_0) \int \psi^* \psi \, dx \\ &\sim \partial_{x_0} V(x_0), \\ \langle \hat{x} \rangle &\sim x_0.\end{aligned}$$

In the Heisenberg picture, the wavepacket does not spread so that equation 5.40 gives the classical equation of motion for the expectation value of the wavepacket. However, the uncertainty in $\hat{x}$ grows with time so that the probability of finding the particle at the centre of mass of the wavepacket, x_0 can be quite small. In the Schrödinger picture the loss of classical behaviour is manifested in the wavepacket spreading. Unfortunately, wavepacket spreading is an extremely rapid process and the period of time for which the behaviour of the wavepacket is classical is extremely short. A free particle wavepacket, for example, representing an electron will double its width in roughly 10^{-29} seconds. For a particle in a box, the spreading time will be similar, and strongly non–classical behaviour will result very quickly as the spreading wave becomes comparable in size to the box and interferes with itself. There are techniques for using non–spreading wavepackets in semiclassical physics [30], but they are used for the purpose of finding approximate quantum results, and do not say anything about the classical limit.

The transition from quantum to classical mechanics is discussed by Scheininger and Kleber [11]. The wall motion they consider consists of piecewise joinings of the form $L(t) = vt + L_0$, which is a special case of 3.27. Their treatment of the quantum problem is that of chapter 3—they find a one cycle evolution operator in the transformed system—and so they are left with the problem of comparing the one cycle (quantum) mapping with a (classical) mapping between consecutive bounces

(recall chapter 2). The solution to the problem lies in their special choice of $L(t)$, for which a one cycle classical mapping can also be found. Their work has three main aims:

1. To reconcile the different mappings found in the quantum and classical cases.
2. To examine the behaviour of classical phase space areas (ie. to compare a classical ensemble of particles with the corresponding wavefunction).
3. To discuss the effects of the nonlocality of the wavefunction in the classical limit.

The conclusions Scheininger and Kleber draw from their study of the phase space are interesting—they show a correspondence between stationary points of the classical one cycle mapping and wavefunctions with the same momentum. These wavefunctions are nearly recurrent under the one cycle mapping in the large energy limit. They take the large energy limit to be a semiclassical limit and state that the simplest, periodic trajectories in phase space have corresponding, nearly periodic semiclassical states.

The effects of the nonlocality of the wavefunction in the classical limit, their third major topic, is an interesting attempt to discuss the $\hbar \to 0$ limit. Unfortunately, they do not seem to be aware of the classical transformations 5.3 and 5.4. Their failure to distinguish between the momenta in the two coordinate systems leads them to infer the existence of a 'local' momentum, $\tilde{p}$ (which actually corresponds to p), defined in terms of the canonical momentum $\bar{p}$ (which actually corresponds to P), and state that "It is the local momentum $\tilde{p}$ (and not $\bar{p}$) to which the semiclassical limit of the quantum problem corresponds." The mistake that they make is to be unaware of the existence of P and to take $\bar{p}$ to be equivalent to p. In this case, $\tilde{p}$ really would appear to be some kind of nonlocality effect. Their conclusion, however, is trivially true from

the nature of the coordinate transformation, and there is no nonlocality effect of this kind.

Another interesting discussion of the classical limit is made by Karner [16], who examines the stability of the quantum and classical solutions. He makes the interesting point that the choice of boundary conditions (Dirichlet) is not obvious and may be responsible for forcing a certain kind of quantum behaviour. He chooses to work in the coordinate system given by the application of $\hat{U}_1$ (equation 3.5), so that the Schrödinger equation is 3.9. The Hamiltonian which generates this is

$$\hat{H} = \frac{\hat{p}^2}{2mL^2} - \frac{\dot{L}}{2L}[\hat{x}\hat{p} + \hat{p}\hat{x}], \tag{5.41}$$

and it can easily be found classically by the analogous transformation generated by $F_2 = xP/L$. Karner's statement is "that in the case of linear equations of motion [which are generated by the classical form of 5.41], the classical and quantal time evolutions agree." The absence of quantum stochasticity then implies an absence of classical stochasticity. He blames this on the Dirichlet boundary conditions. His mistake is to fail to include the bounces at the boundary in his classical equations of motion. These are strongly nonlinear and are the source of classical chaos in the first place. It is not surprising, then, that a failure to include boundary effects gives non–chaotic behaviour.

It is still interesting to question, however, whether or not Dirichlet boundary conditions are too restrictive to adequately describe the problem. The physically satisfactory way to answer this is to substitute a potential for the walls and examine the behaviour of the wavefunction near the wall. Under the transformations $\hat{U}_1$ and $\hat{U}_2$, a quantum Hamiltonian of the form 5.5 transforms to

$$\hat{H} = \frac{\hat{p}^2}{2m} + L^2(\tau)\hat{V}(x) + \frac{mg(\tau)\hat{x}^2}{2}. \tag{5.42}$$

The most striking feature of this equation is the absence of separable cases; even the

case $g(\tau) =$ constant is nonseparable. Separability can only be regained if the wavefunction is excluded from the region in which $\hat{V}$ is nonzero. The related Hamiltonian,

$$\hat{H}' = \frac{\hat{p}^2}{2m} + L^2(\tau)\hat{V}(x) \tag{5.43}$$

will be examined in order to provide some insight into this. The Schrödinger equation associated with $\hat{H}'$ is

$$\frac{-\hbar^2}{2m}\partial_x^2\Psi + L^2(\tau)V(x)\Psi = i\hbar\partial_\tau\Psi. \tag{5.44}$$

Let $V(x)$ be approximated by

$$V(x) = \begin{cases} V_0 & x < 0 \\ 0 & 0 < x < 1 \\ V_0 & x > 1 \end{cases} \tag{5.45}$$

where V_0 is large. Now let

$$\begin{aligned} \hat{H}' &= \hat{H}^0 + \hat{H}^1 \\ \hat{H}^0 &\equiv \hat{p}^2/2m + L^2(0)\hat{V}(x) \\ \hat{H}^1 &\equiv [L^2(\tau) - L^2(0)]\hat{V}(x). \end{aligned} \tag{5.46}$$

Solutions to

$$\hat{H}^0\psi = i\hbar\partial_\tau\psi \tag{5.47}$$

are

$$\psi_n = \phi_n(x)e^{-iE_n\tau/\hbar}, \tag{5.48}$$

where the ϕ_n are eigenstates of $\hat{H}^0$. A solution to 5.44 can be written in terms of the basis states, ψ_n:

$$\Psi = \sum_n a_n(\tau)\phi_n(x)e^{-iE_n\tau/\hbar}, \tag{5.49}$$

where a_n are expansion coefficients satisfying

$$d_\tau a_k = -\frac{i}{\hbar}\sum_n a_n(\tau)\langle\phi_k|\hat{H}^1|\phi_n\rangle e^{-i(E_n - E_k)\tau/\hbar}. \tag{5.50}$$

For the particular form of the potential, 5.45,

$$\phi_n(x) = \begin{cases} A_n e^{\sqrt{2m(V_0-E_n)}\,x/\hbar} & x < 0 \\ B_n e^{\frac{i}{\hbar}\sqrt{2mE_n}\,x} + C_n e^{-\frac{i}{\hbar}\sqrt{2mE_n}\,x} & 0 < x < 1 \\ D_n e^{-\sqrt{2m(V_0-E_n)}(x-1)/\hbar} & x > 1 \end{cases} \tag{5.51}$$

with

$$\begin{aligned} A_n &= 2B_n\left[1 - i\sqrt{\frac{V_0 - E_n}{E_n}}\right]^{-1} \\ D_n &= 2B_n e^{\frac{i}{\hbar}\sqrt{2mE_n}}\left[1 + i\sqrt{\frac{V_0 - E_n}{E_n}}\right]^{-1} \end{aligned} \tag{5.52}$$

The time evolution of the a_k can now be found

$$\begin{aligned} d_\tau a_k &= -4iV_0\left[L^2(\tau) - L^2(0)\right]\sum_n a_n(\tau)\frac{B_k^* B_n\, e^{-\frac{i}{\hbar}(E_n - E_k)\tau}}{\sqrt{2m(V_0 - E_n)} + \sqrt{2m(V_0 - E_k)}} \\ &\quad \times\left[\frac{1}{(1 - i\sqrt{\frac{V_0-E_k}{E_k}})(1 + i\sqrt{\frac{V_0-E_n}{E_n}})} + \frac{1}{(1 + i\sqrt{\frac{V_0-E_k}{E_k}})(1 - i\sqrt{\frac{V_0-E_n}{E_n}})}\right] \end{aligned} \tag{5.53}$$

The assumption that the walls are rigid is that there is a cutoff, j, such that $E_j \ll V_0$ and such that $a_m = 0$, $\forall\, m > j$. Then

$$d_\tau a_k \sim -4i\frac{\left[L^2(\tau) - L^2(0)\right]}{\sqrt{2mV_0}}\sum_{n\le j} a_n B_k^* B_n\sqrt{E_k E_n}\, e^{-\frac{i}{\hbar}(E_n - E_k)\tau}. \tag{5.54}$$

It is apparent that $d_\tau a_k \propto V_0^{-1/2}$. In the limit $V_0 \to \infty, d_\tau a_k \to 0$ and the ϕ_n become stationary states of the Hamiltonian, $\hat{H}'$. Thus, in the large V_0 limit, 5.42 becomes separable and $L^2(\tau)V(x)$ may be replaced by Dirichlet boundary conditions.

The resonant case, for which a periodic application of an infinitesimal effect can cause unbounded quasienergy growth, has been ignored through all of this. For this case, $V_0 \to \infty$ does not separate the Schrödinger equation. However, the terms $L^2(\tau)\hat{V}(x)$ and $(m/2)g(\tau)\hat{x}^2$ have the same periodicity so that the condition for resonant growth in the Fermi–Ulam Accelerator will be satisfied by the quadratic potential

if it is satisfied by the 'wall' potential (recall that the condition is given by 3.26). The quadratic potential, however, will be the dominant source of the resonant growth, and the error in ignoring the boundary effects, and using Dirichlet conditions, will be small.

Chapter 6

The Heisenberg Problem

This chapter begins with the introduction of a solution to the Heisenberg equations of motion 4.59 and 4.60. The inspiration for the solution (as for all Heisenberg solutions) lies in the classical solution. The form of the classical solution, however, must be carefully chosen—it cannot depend explicitly on a sequence of turning times, τ_n, because the idea of a turning time is not defined in quantum mechanics. For the special case $g(\tau) = 0$, it is possible to write a solution by taking the Fourier series of the motion,

$$x(\tau) = 1/2 - \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \frac{[1-(-1)^n]}{(n\pi)^2} e^{in\pi(p_0\tau/m + x_0)}. \tag{6.1}$$

Using the notation of chapter 4, the corresponding operator is defined as

$$\hat{x}(\tau) = \hat{I}/2 - \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \frac{[1-(-1)^n]}{(n\pi)^2} e^{in\pi(\hat{P}_0\tau/m + \hat{x}_0)}. \tag{6.2}$$

The method of quantising an operator is not unique and a very good discussion is given by Shewell [31].

It will now be shown that $\hat{x}(\tau)$ satisfies the requirements necessary for it to be an acceptable solution. There are two necessary requirements:

1. It solves the Heisenberg equations of motion,

$$\begin{aligned} i\hbar d_\tau \hat{x} &= [\hat{x}, \hat{H}], \\ \hat{H} &= \hat{\mathcal{H}}/2m. \end{aligned} \tag{6.3}$$

Explicitly substituting 6.2 into the commutator gives

$$\begin{aligned}[\hat{x},\hat{H}] &= -\sum_{\substack{n=-\infty\\ n\neq 0}}^{\infty}\frac{[1-(-1)^n]}{(n\pi)^2}[e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)},\hat{H}] \\ &= -\sum_{\substack{n=-\infty\\ n\neq 0}}^{\infty}\frac{[1-(-1)^n]}{(n\pi)^2}\sum_{j=0}^{\infty}\frac{(in\pi)^j}{j!}[(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)^j,\hat{H}]. \qquad (6.4)\end{aligned}$$

With the identity 4.58, this becomes

$$\begin{aligned}[\hat{x},\hat{H}] &= -\sum_{\substack{n=-\infty\\ n\neq 0}}^{\infty}\frac{[1-(-1)^n]}{(n\pi)^2}\sum_{j=0}^{\infty}\frac{(in\pi)^j}{j!} \\ &\quad\times\sum_{k=0}^{j-1}(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)^k[(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0),\hat{H}](\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)^{j-k-1} \\ &= -(i\hbar/m)\sum_{\substack{n=-\infty\\ n\neq 0}}^{\infty}\frac{[1-(-1)^n]}{(n\pi)^2}\sum_{j=0}^{\infty}\frac{(in\pi)^j}{j!} \\ &\quad\times\sum_{k=0}^{j-1}(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)^k\hat{\mathcal{P}}_0(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)^{j-k-1}. \qquad (6.5)\end{aligned}$$

Further,

$$\begin{aligned}i\hbar d_\tau\hat{x} &= -i\hbar\sum_{\substack{n=-\infty\\ n\neq 0}}^{\infty}\frac{[1-(-1)^n]}{(n\pi)^2}\sum_{j=0}^{\infty}\frac{(in\pi)^j}{j!}d_\tau(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)^j \\ &= -(i\hbar/m)\sum_{\substack{n=-\infty\\ n\neq 0}}^{\infty}\frac{[1-(-1)^n]}{(n\pi)^2}\sum_{j=0}^{\infty}\frac{(in\pi)^j}{j!} \\ &\quad\times\sum_{k=0}^{j-1}(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)^k\hat{\mathcal{P}}_0(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)^{j-k-1}. \qquad (6.6)\end{aligned}$$

From the equations 6.5 and 6.6 it is apparent that the Heisenberg equation, 6.3, is satisfied. The equations 6.5 and 6.6 *would not* have agreed if $\hat{x}$ had been defined as

$$\hat{x}(\tau)=\hat{I}/2-\sum_{\substack{n=-\infty\\ n\neq 0}}^{\infty}\frac{[1-(-1)^n]}{(n\pi)^2}e^{in\pi(\hat{p}_0\tau/m+\hat{x}_0)}. \qquad (6.7)$$

2. The operator, $\hat{x}(\tau)$ is self adjoint. This will be shown in several steps. First, it should be recalled from chapter 4 that $\mathbf{D}(\hat{\mathcal{P}}_0)=\{f|f(0)=f(1)=0\}$. Further,

it is easily seen that $\mathbf{D}(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0) = \mathbf{D}(\hat{\mathcal{P}}_0)$. The exponential operators in 6.2 are defined by their Taylor series, so that all powers of $\hat{\mathcal{P}}_0\tau/m + \hat{x}_0$ must be defined for the exponential operators to be defined. This gives

$$\mathbf{D}(e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)}) = \{f|(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0)^j f|_{x=0} = (\hat{\mathcal{P}}_0\tau/m + \hat{x}_0)^j f|_{x=1} = 0, \forall j\}. \tag{6.8}$$

This domain is not so restrictive as it might appear—the domain is dense in the Hilbert space and the operator, $\hat{x}$, is bounded (as will be shown next) so that the domain can be extended. Now, consider the operator

$$\hat{e}(n) \equiv e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)} + e^{-in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)}. \tag{6.9}$$

Then

$$\hat{x} = 1/2 - \sum_{n=1}^{\infty} \frac{[1-(-1)^n]}{(n\pi)^2}\hat{e}(n). \tag{6.10}$$

The operator, $\hat{e}(n)$, can easily be shown to be Hermitian. Starting with the Taylor expansion for the exponential operator it can be shown that, for f, h in $\mathbf{D}(\exp[in\pi(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0)])$,

$$\begin{aligned}
\int_0^1 f^* e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)} h\, dx &= \sum_{j=0}^{\infty} \frac{(in\pi)^j}{j!} \int_0^1 f^*(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0)^j h\, dx \\
&= \sum_{j=0}^{\infty} \frac{(in\pi)^j}{j!} \Big\{ -i\hbar f^*(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0)^{j-1} h \Big|_0^1 \\
&\quad -i\hbar[(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0)f]^*(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0)^{j-2} h \Big|_0^1 - \ldots \\
&\quad -i\hbar[(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0)^{j-1} f]^* h \Big|_0^1 \\
&\quad + \int_0^1 [(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0)^j f]^* h\, dx \Big\} \\
&= \int_0^1 [e^{-in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)} f]^* h\, dx
\end{aligned} \tag{6.11}$$

where 6.8 has been used to eliminate the extra terms in the last step of 6.11. From this it follows that $\hat{e}(n)$ is Hermitian. Further, it is obvious from 6.10 that

$\hat{x}$ is Hermitian. Next it can be shown that $\hat{e}(n)$ is bounded. First it is shown that $\exp[in\pi(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0)]$ preserves the norm of a function:

$$\begin{aligned} \|e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)}f\|^2 &= \langle e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)}f|e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)}f\rangle \\ &= \langle e^{-in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)}e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)}f|f\rangle \\ &= \|f\|^2, \end{aligned}$$

where 6.11 has been used. From this it follows that $\hat{e}(n)$ is bounded. Equation 6.10 is a convergent series of bounded operators so that $\hat{x}$, too, is bounded. It should be remarked that even though $\exp[in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)]$ is norm preserving, it is *not* unitary, since $\hat{\mathcal{P}}_0\tau/m + \hat{x}_0$ is not self adjoint

Finally, it is straightforward to show that both $\hat{e}(n)$ and $\hat{x}$ are self adjoint. The domain of a dense, bounded operator can always be extended (as described in chapter 4) to include the entire Hilbert space. Then equation 6.8 can be extended to

$$\mathbf{D}(\hat{e}(n)) = \mathbf{D}(\hat{x}) = \mathbf{H}.$$

Now, if $\langle\phi|\hat{e}(n)h\rangle = \langle f|h\rangle$, for $\phi, f \in \mathbf{H}$ and $h \in \mathbf{D}(\hat{e}(n))$ then

$$\begin{aligned} &\phi \in \mathbf{D}(\hat{e}(n)) \quad \text{(trivially)} \\ &\hat{e}(n)\phi = f \qquad \text{(since } \hat{e}(n) \text{ is Hermitian).} \end{aligned}$$

From the definition of self adjointness, equation 4.7, it follows that $\hat{e}(n)$ is self adjoint. An identical argument will show that $\hat{x}(\tau)$ is also self adjoint. It should be remembered that the important feature of self adjointness is the existence of a complete set of eigenfunctions with real eigenvalues.

The connection between equation 6.2 and the equations of motion 4.59–4.61 needs to be made. Equation 4.59 gives a definition of $\hat{\mathcal{P}}$.

$$\hat{\mathcal{P}} = md_\tau\hat{x}$$

$$= -i \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \frac{[1-(-1)^n]}{n\pi} e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)}\hat{\mathcal{P}}_0$$

$$-i\hbar/2 \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n] e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)} \tag{6.12}$$

Equation 6.12 is just a reordering of 6.6. First it can be shown that, at $\tau = 0$, $\hat{P}$ agrees with the definition 4.8. It is obvious from 6.12 that

$$\begin{aligned} \mathbf{D}(\hat{\mathcal{P}}(0)) &= \{f | f(0) = f(1) = 0\} \\ &= \mathbf{D}(\hat{\mathcal{P}}_0). \end{aligned} \tag{6.13}$$

With this choice of domain, the second term in 6.12 becomes the zero operator: Consider any two functions $f, h \in \mathbf{D}(\hat{\mathcal{P}}(0))$. Then

$$\begin{aligned} &\langle f^* | \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n] e^{in\pi x} | h \rangle \\ &= \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n] \int_0^1 e^{in\pi x} f^* h \, dx \\ &= \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n] \left\{ \frac{e^{in\pi x}}{in\pi} f^* h \Big|_0^1 - \int_0^1 \frac{e^{in\pi x}}{in\pi} d_x(f^* h)\, dx \right\} \end{aligned} \tag{6.14}$$

The sum in 6.14 is

$$\sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n] \frac{e^{in\pi x}}{in\pi} = \begin{cases} -1 & -1 < x < 0 \\ 0 & x = 0, x = 1 \\ 1 & 0 < x < 1 \end{cases} \tag{6.15}$$

and is periodically continued along the real axis.The behaviour at the points $x = 0$ and $x = 1$ in 6.15 cause the first term in 6.14 to vanish identically. The remaining integral, however, is not affected by the discontinuities in 6.15 and is

$$\int_0^1 \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \frac{[1-(-1)^n]}{in\pi} e^{in\pi x} d_x(f^* h)\, dx = (f^* h)\Big|_0^1. \tag{6.16}$$

This vanishes because of 6.13. From the fact that f, h are *arbitrary* elements of $\mathbf{D}(\hat{\mathcal{P}}(0))$, and that $\mathbf{D}(\hat{\mathcal{P}}(0))$ is *dense*, it follows that

$$\sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n] e^{in\pi\hat{x}} = 0. \tag{6.17}$$

With 6.17 and 6.15, 6.12 becomes (at $\tau = 0$)

$$\hat{\mathcal{P}}(0) = \hat{\mathcal{P}}_0. \tag{6.18}$$

The importance of the boundary conditions in determining the behaviour of the solution is hinted at in this calculation.

A similar calculation which is more revealing is one that shows that $d_\tau \hat{\mathcal{P}}|_{\tau=0} = 0$. Equation 4.60 requires that any solution for $\hat{\mathcal{P}}$ have a vanishing time derivative at all times, but at this point a proof has only been found for the case $\tau = 0$. Starting with 6.12, $d_\tau \hat{\mathcal{P}}$ is

$$\begin{aligned} d_\tau \hat{\mathcal{P}} \;=\; & \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n]\, e^{i\hbar(n\pi)^2\tau/2m}\, e^{in\pi x}\, e^{in\pi\hat{\mathcal{P}}_0\tau/m}\, \hat{\mathcal{P}}_0^2/m \\ & +(\hbar/m) \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n](n\pi)\, e^{i\hbar(n\pi)^2\tau/2m}\, e^{in\pi x}\, e^{in\pi\hat{\mathcal{P}}_0\tau/m}\, \hat{\mathcal{P}}_0 \\ & +(\hbar^2/4m) \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n](n\pi)^2\, e^{i\hbar(n\pi)^2\tau/2m}\, e^{in\pi x}\, e^{in\pi\hat{\mathcal{P}}_0\tau/m} \end{aligned} \tag{6.19}$$

The exponential operator has been rewritten with the identity

$$e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)} = e^{i\hbar(n\pi)^2\tau/2m} e^{in\pi x} e^{in\pi\hat{\mathcal{P}}_0\tau/m}$$

(see [31]). The first term in 6.19 is the Fourier expansion for

$$2\sum_{j=-\infty}^{\infty} \left[\delta(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0 - 2j\hat{I}) - \delta((2j+1)\hat{I} - (\hat{\mathcal{P}}_0\tau/m + \hat{x}_0))\right],$$

while the remaining two terms are derivatives of this. Equation 6.19 is divergent and only makes sense in an integration. The domain of 6.19 is

$$\mathbf{D}(d_\tau\hat{\mathcal{P}}) = \{f | f(0) = f(1) = 0, d_x f|_0 = d_x f|_1 = 0\}. \tag{6.20}$$

The three terms in 6.19 will be shown to vanish (at $\tau = 0$) one at a time. The method used here is very similar that used to show 6.18. The first term in 6.19 is dealt with first. For any $f, h \in \mathbf{D}(d_\tau \hat{\mathcal{P}})$,

$$\sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n] \int_0^1 f^* e^{in\pi x} \hat{\mathcal{P}}_0^2 h \, dx =$$

$$\sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n] \left\{ \frac{e^{in\pi x}}{in\pi} [f^* \hat{\mathcal{P}}_0^2 h] \Big|_0^1 - \int_0^1 \frac{e^{in\pi x}}{in\pi} d_x [f^* \hat{\mathcal{P}}_0^2 h] \, dx \right\}, \qquad (6.21)$$

at $\tau = 0$. The first term in 6.21 vanishes identically because of 6.15. The remaining integral is not, however, affected by the discontinuities in 6.15 and is

$$\begin{aligned} \int_0^1 \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n] \frac{e^{in\pi x}}{in\pi} d_x [f^* \hat{\mathcal{P}}_0^2 h] \, dx &= f^* \hat{\mathcal{P}}_0^2 \, h \Big|_0^1 \\ &= 0. \end{aligned} \qquad (6.22)$$

Equation 6.20 has been used to show that this vanishes. Similarly, for the second term in 6.19,

$$\sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n] n\pi \int_0^1 f^* e^{in\pi x} \hat{\mathcal{P}}_0 h \, dx =$$

$$\sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n] n\pi \left\{ \frac{e^{in\pi x}}{in\pi} [f^* \hat{\mathcal{P}}_0 h] \Big|_0^1 - \frac{e^{in\pi x}}{(in\pi)^2} d_x [f^* \hat{\mathcal{P}}_0 h] \Big|_0^1 \right.$$

$$\left. + \int_0^1 \frac{e^{in\pi x}}{(in\pi)^2} d_x^2 [f^* \hat{\mathcal{P}}_0 h] \, dx \right\}. \qquad (6.23)$$

The first term in 6.23 vanishes because of 6.20. The second term vanishes identically because of 6.15 and the third term is

$$\begin{aligned} \int_0^1 \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n] \frac{e^{in\pi x}}{n\pi} d_x^2 [f^* \hat{\mathcal{P}}_0 h] \, dx &= d_x [f^* \hat{\mathcal{P}}_0 h] \Big|_0^1 \\ &= 0. \end{aligned} \qquad (6.24)$$

Finally, for the third term in 6.19,

$$\sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n](n\pi)^2 \int_0^1 e^{in\pi x}[f^*h]\,dx =$$

$$\sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} [1-(-1)^n](n\pi)^2 \left\{ \frac{e^{in\pi x}}{in\pi}[f^*h]\Big|_0^1 - \frac{e^{in\pi x}}{(in\pi)^2} d_x[f^*h]\Big|_0^1 + \frac{e^{in\pi x}}{(in\pi)^3} d_x^2[f^*h]\Big|_0^1 \right.$$

$$\left. - \int_0^1 \frac{e^{in\pi x}}{(in\pi)^3} d_x^3[f^*h]\,dx \right\}$$

$$= 0. \tag{6.25}$$

It follows from equations 6.22, 6.24 and 6.25, the fact that $\mathbf{D}(d_\tau \hat{\mathcal{P}})$ is dense, and the arbitrariness of f and h, that

$$d_\tau \hat{\mathcal{P}}|_{\tau=0} = 0, \tag{6.26}$$

as required.

A simple way of understanding the above calculation is to realise that 6.26 is a statement that all the matrix elements of 6.19 vanish. The choice of boundary conditions is critical in this calculation; if 6.19 had been written with $\hat{p}_0$ taking the place of $\hat{\mathcal{P}}_0$, then 6.22, 6.24 and 6.25 would not have vanished. This is a very clear demonstration of the difference between the statements

$$d_\tau \hat{\mathcal{P}} = 0$$

(recall equation 4.60) and

$$d_\tau \hat{p} = 0$$

(recall equation 4.61). The first of these equations allows $\hat{\mathcal{P}}$ to account for the boundaries (as has just been shown). There is, however no solution for $\hat{p}$ which will account for the boundaries and still satisfy the second equation. The indifference of $\hat{p}$ to the walls is in keeping with the discussion at the end of chapter 4, in which $\hat{p}$ was identified as corresponding to the canonical momentum.

One final calculation involving this solution will be included in this chapter for the sake of completeness. The commutator, $[\hat{x}, \hat{\mathcal{P}}]$, is found:

$$\begin{aligned}
[\hat{x}, \hat{\mathcal{P}}] &= i \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \sum_{\substack{j=-\infty \\ j\neq 0}}^{\infty} \frac{[1-(-1)^n]}{(n\pi)^2} \frac{[1-(-1)^j]}{j\pi} e^{ij\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)} [e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)}, \hat{\mathcal{P}}_0] \\
&= i\hbar \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \sum_{\substack{j=-\infty \\ j\neq 0}}^{\infty} \frac{[1-(-1)^n]}{n\pi} \frac{[1-(-1)^j]}{j\pi} e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)} e^{ij\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)}
\end{aligned}$$

where equations 6.2 and 6.12, and

$$[e^{in\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)}, e^{ij\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)}] = 0$$

have been used. Define $p = n + j$ so that

$$\begin{aligned}
[\hat{x}, \hat{\mathcal{P}}] &= -i\hbar \sum_{p=-\infty}^{\infty} \sum_{\substack{n=-\infty \\ n\neq 0,p}}^{\infty} \frac{[1-(-1)^n]}{n\pi} \frac{[1-(-1)^{p-n}]}{(p-n)\pi} e^{ip\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)} \\
&= -i\hbar \sum_{\substack{p=-\infty \\ p\neq 0}}^{\infty} \sum_{\substack{n=-\infty \\ n\neq 0,p}}^{\infty} \frac{[1-(-1)^n][1+(-1)^p]}{p\pi} \left[\frac{1}{n\pi} + \frac{1}{(p-n)\pi}\right] e^{ip\pi(\hat{\mathcal{P}}_0\tau/m+\hat{x}_0)} \\
&\quad +2i\hbar \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \frac{[1-(-1)^n]}{(n\pi)^2}.
\end{aligned}$$

The sum over n in the first term is zero so that

$$\begin{aligned}
[\hat{x}, \hat{\mathcal{P}}] &= 2i\hbar \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \frac{[1-(-1)^n]}{(n\pi)^2} \\
&= i\hbar \qquad (6.27)
\end{aligned}$$

This is not surprising since $\hat{\mathcal{P}}$ is not very much different from a momentum operator.

The chapter will be concluded with the discussion of a phenomenological approach to the quantum Fermi–Ulam Accelerator, which has been proposed by Razavy [32]. For the case $g(\tau) = 0$, the classical Hamiltonian is chosen to be

$$\begin{aligned}
H &= \frac{p^2}{2m}\vartheta(x) \\
\vartheta &= [2\theta(x)-1][2\theta(1-x)-1], \qquad (6.28)
\end{aligned}$$

where $\theta(x)$ is the step function. In the interval $0 < x < 1$, 6.28 has the form of a free particle Hamiltonian. The function $\vartheta(x)$ has been chosen such that a particle will be contained within the interval. This is obvious from the equations of motion

$$\begin{aligned} d_\tau x &= \partial_p H \\ &= \frac{p}{2m}\vartheta(x) \qquad (6.29) \\ d_\tau p &= -\partial_x H \\ &= -\frac{p^2}{2m} d_x \vartheta(x) \qquad (6.30) \end{aligned}$$

Differentiating 6.29 with respect to time and using 6.30 to eliminate $d_\tau p$ gives

$$\begin{aligned} d_\tau^2 x &= -\frac{p^2}{2m^2}\vartheta\, d_x\vartheta + \frac{p}{m} d_\tau x\; d_x\vartheta \\ &= \frac{d_x\vartheta}{2\vartheta}(d_\tau x)^2. \qquad (6.31) \end{aligned}$$

This can be integrated once to give

$$d_\tau x = \pm C\sqrt{\vartheta(x)} \qquad (6.32)$$

where C is a constant of integration. Then p is (from 6.29)

$$p = \pm\frac{mC}{\sqrt{\vartheta(x)}}. \qquad (6.33)$$

From 6.32 it is clear that $x = 0$ and $x = 1$ are turning points since $d_\tau x$ is only real valued inside $[0, 1]$. Outside $[0, 1]$, $d_\tau x$ is imaginary. The same kind of behaviour can be observed in a potential well in which $d_\tau x = \pm\sqrt{2(E - V(x))/m}$. From 6.33 it is clear that p is the mechanical momentum in the region $0 < x < 1$, but diverges at the endpoints.

The Hamiltonian is quantised:

$$\begin{aligned} H &= \frac{1}{8m}\left[\vartheta(\hat{x})\hat{p}^2 + 2\hat{p}\vartheta(\hat{x})\hat{p} + \hat{p}^2\vartheta(\hat{x})\right] \\ &= \frac{1}{2m}\left[\vartheta(\hat{x})\hat{p}^2 - i\hbar d_x\vartheta(\hat{x})\hat{p} - \frac{\hbar^2}{4} d_x^2\vartheta(\hat{x})\right]. \qquad (6.34) \end{aligned}$$

This form is not unique [31], but other choices will differ by terms of order $\hbar^2$. Equation 6.34 gives the equations of motion

$$\begin{aligned} d_\tau \hat{x} &= \left[\frac{\vartheta(\hat{x})\hat{p} + \hat{p}\vartheta(\hat{x})}{2m}\right] \\ &= \left[\frac{\vartheta(\hat{x})\hat{p}}{m} - \frac{i\hbar}{2m} d_x \vartheta(\hat{x})\right] \end{aligned} \tag{6.35}$$

$$d_\tau \hat{p} = -\frac{1}{2m}\left[d_x\vartheta(\hat{x})\hat{p}^2 - i\hbar\left(d_x^2\vartheta(\hat{x})\right)\hat{p} - \frac{\hbar^2}{4} d_x^3 \vartheta(\hat{x})\right]. \tag{6.36}$$

Here, $\hat{p}$ is obviously different from the canonical momentum operator which is used throughout the earlier chapters. However, at $\tau = 0$

$$\hat{p}(0) = -i\hbar\partial_x \tag{6.37}$$

$$\hat{x}(0) = x \tag{6.38}$$

Using these two equations, and the Hamiltonian given in 6.34, the Schrödinger equation is

$$E\psi = -\frac{\hbar^2}{2m}\left[\vartheta d_x^2\psi + d_x\vartheta\, d_x\psi + \frac{1}{4} d_x^2\vartheta\, \psi\right] \tag{6.39}$$

This equation is just the free particle Schrödinger equation in the region $0 < x < 1$. Furthermore, the last term on the right forces the boundary conditions $\psi(0) = \psi(1) = 0$. This can be shown if equation 6.39 is integrated once. Let x_1 be in the interval. Then

$$\begin{aligned} \int_{x_1}^{x} E\psi\, d_x = -\frac{\hbar^2}{2m}\Bigg[&\int_{x_1}^{x} \vartheta d_x^2\psi\, d_x + \int_{x_1}^{x} d_x\vartheta\, d_x\psi\, d_x + \frac{1}{4} d_x\vartheta\, \psi\Big|_{x_1}^{x} \\ &- \frac{1}{4}\int_{x_1}^{x} d_x\vartheta\, d_x\psi\, d_x\Bigg] \end{aligned} \tag{6.40}$$

The term

$$\frac{1}{4} d_x\vartheta\, \psi\Big|_{x_1}^{x}$$

is badly behaved in the limits $x \to 0$ and $x \to 1$ unless ψ goes to zero quite strongly. The left side of equation 6.40 should be continuous for physical reasons, however. From this it follows that ψ must vanish at the endpoints of the box.

It is instructive to compare equation 6.35 with equation 6.12. Equation 6.12 may be written as

$$d_\tau \hat{x} = \vartheta'(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0)\,\hat{\mathcal{P}}_0 - \frac{i\hbar}{2m}\,d_x\left[\vartheta'(\hat{\mathcal{P}}_0\tau/m + \hat{x}_0)\right]. \tag{6.41}$$

The function $\vartheta'(x)$ is similar to $\vartheta(x)$ but is periodically continued along the real axis:

$$\vartheta'(x) = \begin{cases} 1 & 2j < x < 2j+1 \\ 0 & x = \ldots -1, 0, 1 \ldots \\ -1 & 2j+1 < x < 2j+2 \end{cases} \tag{6.42}$$

where j is any integer. Classically the difference between 6.41 and 6.35 is clear. $p_0\tau/m + x_0$ is the total distance travelled by the particle, while x is the displacement of the particle. The function $\vartheta'(p_0\tau/m + x_0)$ is alternately $+1$ and -1 depending on the distance the particle has travelled. The initial momentum, p_0, is a constant so that the combination $\vartheta'(p_0\tau/m + x_0)p_0$ changes sign as the particle bounces from the walls. In the combination $\vartheta(x)p$, however, the function $\vartheta(x)$ is always $+1$ and it is p that changes sign as the particle strikes the walls. Thus, the combinations $\vartheta'(p_0\tau/m + x_0)p_0$ and $\vartheta(x)p$ generate the same classical behaviour, and equations 6.35 and 6.41 are the quantum analogues of two different classical descriptions of the same system.

The case of the quantum Fermi–Ulam Accelerator with nonzero g can now be formulated. The Hamiltonian is

$$H = \frac{1}{2m}\left[\vartheta(\hat{x})\hat{p}^2 - i\hbar\, d_x\vartheta(\hat{x})\,\hat{p} - \frac{\hbar^2}{4}d_x^2\vartheta(\hat{x})\right] + \frac{m}{2}g(\tau)x^2. \tag{6.43}$$

The equations of motion are

$$d_\tau \hat{x} = \left[\frac{\vartheta(\hat{x})\hat{p}}{m} - \frac{i\hbar}{2m}\,d_x\vartheta(\hat{x})\right] \tag{6.44}$$

$$d_\tau \hat{p} = -\frac{1}{2m}\left[d_x\vartheta(\hat{x})\hat{p}^2 - i\hbar\, d_x^2\vartheta(\hat{x})\,\hat{p} - \frac{\hbar^2}{4}d_x^3\vartheta(\hat{x})\right] - mg(\tau)\hat{x} \tag{6.45}$$

and Dirichlet boundary conditions still apply.

Chapter 7

Summary and Conclusion

The most impressive thing which has been demonstrated in this thesis is just how complicated the Heisenberg approach to the particle–in–a–box problem is. The Schrödinger approach is simple enough to be the second example (after the free particle) discussed in any introductory quantum mechanics course. The classical problem is too trivial to even make it into a classical mechanics course. There are three points which contribute to the difficulty of working in the Heisenberg picture:

1. Quantum operators must be self adjoint. Self adjointness is really a statement about the domain of the operator. The first consequence of self adjointness is that expectation values of the operator will be real. The need for this is obvious since the expectation values correspond to physically observed quantities. The second consequence of self adjointness is that a complete set of eigenstates of the operator exists. The importance of this point is not so obvious, and yet the consequences are far reaching. The eigenstates of an operator provide an important basis set in terms of which quantum states may be represented. The behaviour of the state is crucially dependent on the choice of basis set, a point which is made clear in the comparison of $\hat{p}^2$ and $\hat{\mathcal{H}}$ in chapter 4. It is interesting to notice that if the domain of $\hat{\mathcal{H}}$ had been the entire Hilbert space, then $\hat{\mathcal{H}}$ could not have represented a physical quantity: there would be a choice of basis sets, both of which would generate different physical behaviour. The condition of self adjointness guarantees an unambiguous choice of basis states with which to work.

The effects of self adjointness on the Heisenberg equations of motion are subtle. This is demonstrated in chapters 4 and 6 where the behaviour of the operators $\hat{p}$ and $\hat{\mathcal{P}}$ is compared. Here, again, the difference in behaviour is directly attributable to the domain of the operators. In chapter 4 it is shown how the choice of Hamiltonian disallows solutions for $\hat{x}$ which ignore the boundaries, while in chapter 6 it is shown that a solution which incorporates boundary effects *is* a solution. A very careful definition of the operators involved is essential to ensure that a solution to the Heisenberg equations is correct.

2. A solution to the Heisenberg equations must be found. Generally, if a solution for the classical problem can be found then there is an algorithmic method of generating the operator behaviour [31]. The classical equations of motion are nonlinear, however, and tend to be more difficult to solve than the corresponding Schrödinger equation. Furthermore, the form of the solution must be very carefully chosen—it cannot consist of a number of separate solutions joined by hand, which is the usual approach for dealing with a discontinuity in a classical system. This poses a problem for the quantum Fermi–Ulam Accelerator, where the classical solution is joined at every bounce. In the very simplest case, dealt with in chapter 6, a solution is possible because the classical motion is periodic, and the classical motion may be written as a Fourier series. The example studied in chapter 6 is for the case $g(\tau) = 0$. The case $g(\tau) =$ constant also yields periodic classical solutions. The problem with quantising this is that there are two types of classical solution depending on the energy of the particle (the turning points are at the walls at the higher energies and fall short of the walls at lower energies). This problem may not be insurmountable.

3. It must be possible to calculate physical quantities with the solution. One of the major difficulties in working with $\hat{x}(\tau)$ is finding a set of orthogonal states which form a complete basis. This is hinted at in chapter 4, where it is shown

that $\hat{\mathcal{P}}_0\tau/m + \hat{x}_0$ has no eigenstates.

With all the difficulties inherent in the Heisenberg approach, it is reasonable to ask why the problem is worth undertaking. The most intriguing feature of the Heisenberg approach is its closeness to the classical solution. Operator solutions differ from their classical counterparts by terms of order $\hbar$ or higher. They provide a much closer link to classical mechanics than does the Schrödinger formalism. For this reason, the Heisenberg formalism may be able to provide better insight into the semiclassical limit than the Schrödinger picture has in the past. In particular, the problem of comparing classical stochasticity with the quantum behaviour in the quantum Fermi–Ulam Accelerator seems to lend itself to the Heisenberg formulation. Another problem which is worth studying in terms of the Heisenberg formulation is the phenomenon of quantum resonance (recall the discussion in chapter 3). Here, it seems that the terms proportional to powers of $\hbar$ in the operator solutions *dominate* the classical terms so that an effect with no classical counterpart is obtained.

The solution to the Heisenberg equations of motion presented in chapter 6 is obviously not complete. A complete set of eigenstates needs to be found, and the proof that $\hat{\mathcal{P}}$ satisfies the equations of motion for all times needs to be found. The next goal would be to extend the solution to the case where $g(\tau)$ is piecewise constant. Such a system exhibits both regular and stochastic behaviour and lends itself to a comparison of the quantum and classical evolutions. The work of chapter 5 provides a starting point for studies of the semiclassical regime. The interesting question is how the spectrum of the Hamiltonian manifests itself in the behaviour of the Heisenberg operators. The alternative formulation of the problem, presented in chapter 6, also requires more study. The hope is that it might provide a simpler method for finding solutions. Less immediate avenues of research include understanding why a classical solution must be of a specific form before it can be quantised, discovering how to

formulate the semiclassical limit for systems in which the time dependence cannot be removed and investigating whether a similar kind of treatment can be made of some of the time independent systems which are popular in quantum chaology.

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